PB86-187770

Guidelines for Using OZIPM-3 with CBM-X or Optional Mechanisms. Volume 1 Description of the Ozone Isopleth Plotting Package, Version 3

Systems Applications, Inc., San Rafael, CA

Prepared for

Environmental Protection Agency
Research Triangle Park, NC

Jan 86

U.S. Department of Commerce
National Technical Information Service
NTIS

PB86-187770

EPA/600/3-86/004a
January 1986

GUIDELINES FOR USING OZIPM-3 WITH CBM-X OR OPTIONAL MECHANISMS

Volume 1.

Description of the Ozone Isopleth Plotting Package/ Version 3

by

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REPRODUCED BY
NATIONAL TECHNICAL
INFORMATION SERVICE
U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA

(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA/600/3-86/004a

2. EPA/SW/MT-86/018a

3. RECIPIENT'S ACCESSION NO. PB86-187770/AS

4. TITLE AND SUBTITLE

GUIDELINES FOR USING OZIPM-3 WITH CBM-X OR OPTIONAL MECHANISMS

Volume 1/Version 3

5. REPORT DATE January 1986

6. PERFORMING ORGANIZATION CODE

7. AUTHOR(S) H. Hogo and G. Z. Whitten

8. PERFORMING ORGANIZATION REPORT NO.

9. PERFORMING ORGANIZATION NAME AND ADDRESS

Systems Applications, Inc.
101 Lucas Valley Road
San Rafael, CA 94903

10. PROGRAM ELEMENT NO. CDWA1A/01-1130(FY-85)

11. CONTRACT/GRANT NO. Contract 68-02-3735

12. SPONSORING AGENCY NAME AND ADDRESS

Atmospheric Sciences Research Laboratory-RTP, NC
Office of Research and Development
U.S. Environmental Protection Agency
Research Triangle Park, North Carolina 27711

13. TYPE OF REPORT AND PERIOD COVERED Final (8/82 - 7/85)

14. SPONSORING AGENCY CODE EPA/600/09

15. SUPPLEMENTARY NOTES

for magnetic tape see PB86-187788

16. ABSTRACT

A computer program, called Ozone Isopleth Plotting with Optional Mechanisms/Version 3 (OZIPM-3), has been developed. The program enables the use of a new Carbon Bond Mechanism (CBM-X) for EKMA control strategy calculations. The OZIPM-3 program also has the capability to accept a chemical mechanism other than the default CBM-X that is internally stored in the program. Volume 1 serves as the User's Manual for OZIPM-3. It contains a detailed description of how OZIPM-3 operates. It also contains a thorough discussion of the different input and output options available to the user when exercising either the default CBM-X mechanism or an optional mechanism. Five examples of OZIPM-3 simulations are presented. Input and output files for each example are included.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group

18. DISTRIBUTION STATEMENT

RELEASE TO PUBLIC

19. SECURITY CLASS *(This Report)* UNCLASSIFIED

20. SECURITY CLASS *(This page)* UNCLASSIFIED

21. NO. OF PAGES 253

22. PRICE $29.95

EPA Form 2220-1 (9-73)

NOTICE

The information in this document has been funded by the United States Environmental Protection Agency under Contract No. 68-02-3735 to Systems Applications, Inc. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document.

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ABSTRACT

The U.S. Environmental Protection Agency is continuing to recommend the use of the Empirical Kinetic Modeling Approach (EKMA) as a procedure for relating levels of photochemical ozone to levels of organic compounds and oxides of nitrogen. In a recent study, Systems Applications developed a new chemical mechanism that is suitable for use in EKMA. The mechanism, called the extended Carbon-Bond Mechanism (CBM-X), provides the most up-to-date and verified description of urban smog chemistry currently available. In the study reported here, a new computer program called Ozone Isopleth Plotting with Optional Mechanisms--Version 3 (OZIPM-3) was developed to enable the use of the CBM-X mechanism for EKMA control strategy calculations. The OZIPM-3 program can also use a chemical mechanism other than the default CBM-X that is internally stored in the program. Volume 1 serves as the User's Manual for OZIPM-3. It contains both a detailed description of how OZIPM-3 operates and a thorough discussion of the different input and output options available to the user when exercising either the default CBM-X mechanism or an optional mechanism. Five examples of OZIPM-3 simulations and input and output files for each example are included. Volume 2 contains the FORTRAN listing of the computer code. A magnetic tape of this code is also available. OZIPM-3 expands on earlier codes by providing a wider compatibility between computers, a feature that allows calculation of control strategies without drawing an isopleth diagram, and easier input for photolysis rates when optional chemical mechanisms are used.

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SECTION 1

OVERVIEW

BACKGROUND AND PURPOSE

The U.S. Environmental Protection Agency (EPA) has defined three levels of modeling to be used in the formulation of State Implementation Plans (SIPs). Level III consists of a city-specific Empirical Kinetic Modeling Approach (EKMA) used in accordance with a guideline document issued in March 1981 (EPA, 1981). Level II refers to the use of EKMA with more complex two-dimensional models, and Level I refers to the use of large, sophisticated air quality simulation models (AQSMs) such as the Systems Applications Urban Airshed Model.

EKMA was developed as a procedure for relating levels of photochemical oxidants (expressed as ozone) to levels of organic compounds and oxides of nitrogen (EPA, 1977); it utilizes a set of ozone isopleths that depict maximum afternoon concentrations of ozone as a function of the following parameters:

Morning concentrations of nonmethane organic compounds (NMOC) and oxides of nitrogen (NO_x);

Emissions of volatile organic compounds (VOC) and NO_x occurring during the day;

Meteorological conditions; and

Reactivity of the NMOC mix.

The isopleths are developed through computer simulations of atmospheric photochemical reactions using various assumed levels of NMOC and NO_x concentrations. The ozone isopleths are then plotted as a function of initial precursor concentrations. The isopleths are used to compute the percent reduction in NMOC that is needed to lower peak ozone to the National Ambient Air Quality Standard (NAAQS) of 0.12 ppm.

A computer program has been developed that readily generates the ozone isopleths for EKMA users. This program is called the Ozone Isopleth Plotting Package (OZIPP). Detailed documentation of EKMA and OZIPP is given in EPA (1977); Whitten and Hogo (1978a); EPA (1981); and EPA (1984).

Since its origin, more sophisticated versions of the OZIPP model have been developed. Two of these models are

> OZIPM--Version 1--a computer routine with the capability of handling different chemical kinetics mechanisms (Whitten and Hogo, 1978b). This version can be used in Level III analyses.
>
> OZIPM--Version 2--this version of OZIPM contains some code modifications to the original version so that it can be used easily on different computer systems. This version also has the capability of calculating the needed percent reduction in NMOC without first generating an isopleth (Gipson, 1984).

A new mechanism, called the CBM-X, was recently developed and tested against auto exhaust smog chamber data. The results of that work are described in Whitten et al. (1985b). In order to be able to use the CBM-X in EKMA, a new version of OZIPP called OZIPM-3 was developed. The CBM-X is imbedded in this computer routine. The purpose of this document is to provide guidelines on how to exercise the CBM-X (or optional mechanisms selected by the user) in OZIPM-3.

Volume 1 serves as the User's Manual for OZIPM-3. Section 2 of this volume contains an overall technical description of how OZIPM-3 operates. Section 3 presents a detailed description of the different input and output options available to the OZIPM-3 user. Section 4 provides guidance on how to select input options when using the CBM-X stored in OZIPM-3. Section 5 contains a summary of the options discussed in Sections 3 and 4 and serves as a quick reference guide for the User. Section 6 contains examples of model runs. These examples demonstrate the use and flexibility of OZIPM-3. Volume 2 contains the computer code listing for OZIPM-3. A magnetic tape of this program can be purchased from the National Technical Information Service, Springfield, Virginia 22161, telephone (703) 557-4650, or from the principal investigator, Dr. Gary Z. Whitten, Systems Applications, Inc., 101 Lucas Valley Road, San Rafael, California 94903, telephone (415) 472-4011.

The documentation contained in Volume 1 is similar to that contained in the original OZIPP manual (Whitten and Hogo, 1978a). Much of the discussion of concepts and scope of use in the original OZIPP manual applies to OZIPM-3; however, we repeat some of this information here for the sake of completeness. The user of OZIPM-3 is referred to the original OZIPP manual for background discussions.

SCOPE OF USE

Limitations

The OZIPM is limited in applicability to ozone problems within, or immediately downwind of, large urban areas, and thus should not be applied to the following situations unless special attention is given to existing limitations and assumptions:

> The rural ozone problem;
>
> Situations in which transported ozone and/or precursors are clearly dominant (i.e., multiday transport situations);
>
> Cases in which the maximum ozone concentration occurs at night or in the early morning; and
>
> Development of control strategies for single or small groups of emission sources.

The validity of an ozone isopleth diagram generated by OZIPM for a particular city may be limited by the following considerations:

> The kinetic mechanism used to describe the transformations of NMOC and NO_x;
>
> The physical assumptions used to formulate the trajectory model coded into OZIPM;
>
> The meteorological data and assumptions used to specify the parameters required to apply OZIPM;
>
> The availability and reliability of current ozone data, precursor concentration data, and the VOC and NO_x emission inventories;
>
> The mathematical assumptions needed to integrate the differential equations formulated within OZIPM; and
>
> The interpolations needed to generate isopleths from the results of a number of computer simulations.

Because these considerations are part of the basic definitions and concepts that constitute OZIPM and EKMA, they are explained more fully in the following sections.

BASIC DEFINITIONS

Kinetic Mechanism

A kinetic mechanism is a set of chemical reactions and rate constants that is intended to describe some chemical process. Using a kinetic mechanism, one can derive coupled, first-order, ordinary, nonlinear differential equations that describe the rates of change of pollutant concentrations with time. These equations can then be integrated using a computer to simulate the changing pollutant concentrations in a smog chamber or in the atmosphere.

The original version of EKMA (OZIPP) used a two-hydrocarbon/NO_x mechanism to describe the photochemical formation of ozone (Dodge, 1977). In that mechanism, propylene and butane are used as surrogates to represent the urban mix of emissions. The propylene-to-butane ratio of 1:3 in that mechanism cannot be adjusted to account for the changing reactivity of the urban hydrocarbon mix. Because of this and other shortcomings of the original OZIPP program, many users indicated the need for a more flexible chemical mechanism, which was provided by Killus and Whitten (1984) with a version of the Carbon-Bond Mechanism (CBM-3). Very recently, an expanded version of the CBM-3, called the extended Carbon-Bond Mechanism (CBM-X), was developed. This mechanism has now been incorporated in OZIPM-3 as the default chemical mechanism.

Use of a mechanism such as the Extended Carbon-Bond Mechanism (CBM-X) in OZIPM instead of the Dodge propylene/butane mechanism has the following advantages:

(1) The CBM-X is more responsive to a wider range of reactivity than is the Dodge mechanism.

(2) Reactivity is difficult to define as a function of propylene and butane if such reactivity is to be related to changes in the ambient mix of hydrocarbons.

Use of the CBM-X in OZIPM instead of the CBM-3 mechanism has the following potential advantages:

(1) The CBM-X is based on more recent measurements of rate constants.

(2) The CBM-X has been validated with more extensive smog chamber data than has the CBM-3.

It should be noted that the CBM-X is still undergoing additional testing and refinement. This effort will not be completed until late 1987. Until that time, it is recommended that CBM-X be used only as a research tool. We do not advocate the use of CBM-X for SIP development by state and local agencies at this time.

Precursors of Ozone

Precursors of ozone are the chemical species that react to form ozone. The primary precursors are total organic compounds (TOC) and oxides of nitrogen (NO_x). The EPA guidelines (EPA, 1981) on the use of city-specific EKMA contain two definitions of organic compounds. The first definition, termed "VOC" or volatile organic compounds, represents the sum of the reactive organic emissions included in emission inventories. The second definition, termed "NMOC" or nonmethane organic compounds, represents ambient measurements of all organic compounds other than methane. Both VOC and NMOC are precursors of ozone. Methane is not considered a precursor because it reacts very slowly. In this document, organic compounds associated with emission inventories will be termed "VOC". Organic compounds associated with the background and initial concentrations in the surface and aloft layers will be termed "NMOC" because these are typically associated with ambient measurements rather than with emission inventories. NO_x, as used in this report, signifies the sum of the concentrations of nitric oxide (NO) and nitrogen dioxide (NO_2).

Simulation

A computer simulation involves the calculation of the concentrations of pollutants found in the kinetic mechanism as a function of time. Concentrations are calculated at various times specified by the user. The calculations involve the integration of a set of coupled, first-order, nonlinear, ordinary differential equations defined by the kinetic mechanisms that describe the chemical and physical processes underlying the model. User-specified assumptions about initial precursor concentrations, emission patterns, dilution, transported pollutants, reactivity, and light intensity are incorporated in each simulation.

Ozone Isopleth Diagram

An ozone isopleth diagram as generated by OZIPM-3 is illustrated in Figure 1. Each curved line in the diagram represents a constant, maximum, one-hour average ozone concentration. Thus, the NMOC and NO_x coordinates associated with any point on a single, curved line produce the same maximum concentration of ozone. In OZIPM-3, about 60 simulations are normally performed to produce such a diagram.

Reactivity

This is a property of the precursors that governs the rate and extent of ozone production. Each kinetic mechanism that might be used in OZIPM-3 handles this property differently. In general, it is handled by a specific blend of the NMOC species.

Default Values

Certain parameters are needed to run OZIPM-3. The default values are the values of these parameters that will be used unless other values are entered in the input data. For example, the default value for the highest NMOC used in the construction of an isopleth diagram is 2.0 ppmC. If no number is entered in the input data for this parameter, OZIPM-3 will use 2.0 by default.

Diagram Point

Any point on an ozone isopleth diagram generated by OZIPM-3 is associated with three parameters: initial NMOC and NO_x precursor concentrations, and a maximum one-hour average ozone concentration corresponding to the initial NMOC and NO_x concentrations. A set of these three parameters is termed a diagram point. The ozone concentrations at some diagram points are determined from actual computer simulations (i.e., by integrating the set of differential equations). The ozone concentrations at other diagram points are interpolated from the simulated diagram points.

Spline Interpolation

Spline interpolation is used to determine the ozone concentrations between diagram points for which ozone concentrations have been calculated by computer simulations. (Interpolation is used to reduce the number of computer simulations necessary to construct an isopleth diagram

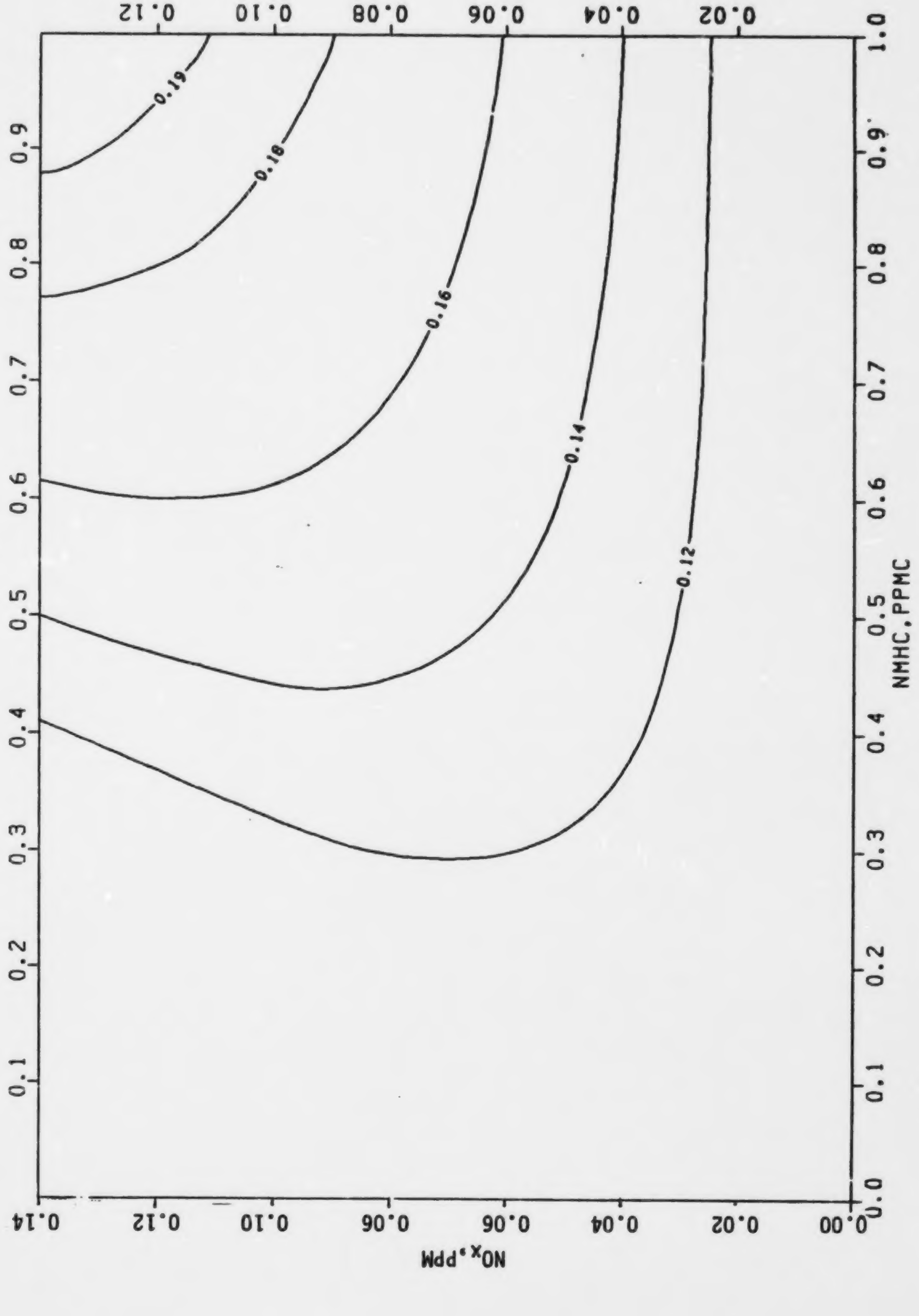

Figure 1. Ozone isopleth diagram generated using the CBM mechanism.

and hence to reduce the cost of running OZIPM.) A spline function is similar to a wire constrained to touch certain points. If the wire is pulled taut, it will bend at each point, but will be straight between points. If the tension is reduced, the wire will provide a smooth curve that touches the points. The hyperbolic spline functions used to interpolate between calculated diagram points in OZIPM have an adjustable tension factor analogous to the tension on a wire. Interpolations are performed internally by the OZIPM, and usually there is no need for the user to be directly concerned with the spline functions.

SUMMARY OF INPUT DATA

Input parameters that can be specified by the user when performing an OZIPM-3 calculation include

Chemical kinetic mechanism;

Zenith-angle-dependence of the photolysis reactions in the chemical mechanism;

Latitude;

Longitude;

Time zone;

Date;

Morning and afternoon mixing heights (also called mixing depths) or hourly mixing depths;

Hourly temperature variation;

The simulation start and stop times;

Concentrations of NMOC, NO_x, ozone, and up to 10 other species in the air above the mixed layer due to transport aloft (note that these cannot be varied in time);

Concentrations of NMOC, NO_x, ozone, and any other chemical species transported in the surface layer;

Background concentrations of NMOC, NO_x, and ozone. The background represents the minimum levels in both the surface layer and aloft that could be achieved if all urban emissions were reduced to zero (i.e., continental background);

VOC and NO_x emissions at each hour;

Organic reactivity. Four reactivities can be specified: background, initial, aloft, and emitted. However, each type of reactivity is fixed in time for each diagram point and at every point on the diagram;

NO_x reactivity (initial fraction of NO_x that is NO_2); and

Surface deposition as a function of time for up to 10 species.

OUTPUT OPTIONS

The major function of OZIPM-3 is to calculate estimated NMOC reductions needed to achieve the ozone air quality standard. The output depends on the option selected by the User. Three types of output can be requested:

(1) Perform a single calculation.

(2) Compute VOC emission reduction for a particular case without generating an O_3 isopleth.

(3) Generate an O_3 isopleth.

SECTION 2

TECHNICAL DISCUSSION

The OZIPM-3 is a trajectory-type model designed to simulate ozone formation in urban atmospheres. The model consists of two distinct parts: the first part is a kinetic mechanism that mathematically simulates the physical and chemical processes taking place in the atmosphere. The second part uses the simulation results to calculate a control strategy for a specific test case or to construct an ozone isopleth diagram. This chapter describes the conceptual basis for the kinetics model and the mathematical techniques used in performing a simulation.

CONCEPTUAL BASIS FOR THE OZIPM-3 KINETIC MECHANISM

In the OZIPM-3 kinetics model, a column of air containing ozone and precursors is transported along an assumed trajectory (either straightline or based on wind patterns). As the column moves, it encounters fresh precursor emissions that are mixed uniformly within the column. The column is assumed to extend from the earth's surface through the mixed layer. The assumed horizontal dimensions of this column are such that the concentration gradients are small enough to make the horizontal exchange of air between the column and its surroundings insignificant. The air within the column is assumed to be uniformly mixed at all times.

At the beginning of a simulation, the column is assumed to contain some specified initial concentrations of NMOC and NO_x. As the column moves along the assumed trajectory, the height of the column can change because of temporal and spatial variations in mixing height; it is assumed to change with time during a user-selected period, and to be constant before and after that period. As the height of the column increases, its volume increases, and air above the inversion layer is mixed in. Pollutants above the mixed layer are described as "transported above the surface layer" or "transported aloft." Any ozone or ozone precursors above the mixed layer that are mixed into the column as it expands are assumed to be rapidly mixed throughout the column.

The kinetics model in OZIPM-3 also considers emissions of VOC and NO_x into the column as it moves along its trajectory. The concentrations of these species within the column are physically decreased by dilution due to the inversion rise, and physically increased both by entrainment of pollutants transported aloft and by fresh emissions. All species react chemically according to the kinetic mechanism selected. Certain photolysis rates within that mechanism are functions of the intensity and spectral distribution of sunlight, and they vary diurnally according to time of year and location.

The following assumptions and specifications describe the OZIPM-3 trajectory model:

> The air mass of interest is an imaginary air parcel (column) of fixed horizontal area at a diurnally varying uniform temperature, within which pollutants are well mixed.
>
> The region of the atmosphere containing the imaginary column is sufficiently homogeneous that horizontal diffusion does not affect pollutant concentrations within the column.
>
> The height of the column varies with time as specified by the user within the options available.
>
> The column contains specified initial concentrations of NMOC and NO_x at the simulation starting time.
>
> Pollutants transported within the surface layer from outside the area of interest may be present in the column at the start of each simulation. The pollutant concentrations due to transport in the surface layer are normally assumed to be zero, but the user may specify other values for the NMOC, NO_x, and ozone concentrations transported within this layer.
>
> The changes in pollutant concentrations within the column are calculated by computer simulation for a user-specified period.
>
> Entrainment of pollutants transported aloft is possible during the rise of the mixed layer. OZIPM-3 permits entrainment of NMOC, NO_x, ozone, and a limited number of other species, but the concentrations in the layer aloft cannot be varied in time.
>
> Pollutants emitted into the column after the starting time can be represented by specifying additions of VOC and NO_x during each hour.
>
> Zero cloud cover is assumed.

Other assumptions relating to the use of EKMA to predict control requirements or changes in urban ozone concentrations as a result of changes in precursor emissions are discussed in EPA (1981).

COMPUTATIONAL PROCEDURES

This section presents a detailed description of the mathematical procedures used in OZIPM to calculate the maximum one-hour average ozone concentration that results from given initial concentrations of NMOC and NO_x. These procedures are based on the physical and chemical processes described in the last section. Before the beginning of a simulation, data-preparation steps are performed by the program. A simulation is conducted by first determining concentrations at the starting time and then numerically integrating the equations that form the basis of the model. The numerical solution yields species concentrations as a function of time continuously throughout the simulation period. The following discussion describes the data-preparation steps, the calculation of initial concentrations, the model formulation, and the numerical integration technique used.

Data-Preparation Steps

Because all simulations performed by OZIPM in generating an ozone isopleth diagram have identical conditions except for the initial NMOC and NO_x concentrations, a data-preparation step is performed by the program before the first simulation begins. The purpose of this step is to eliminate abrupt changes in photolytic rate constants and emission rates. Elimination of these abrupt changes (i.e., discontinuities) is desirable for three reasons:

(1) The integration scheme requires less computer time (discontinuities require the use of small time steps).

(2) The results are more accurate numerically (stepping past discontinuities can lead to errors).

(3) The atmosphere does not normally have discontinuities. (The simulation of intermittent cloud cover or sudden changes in emissions is outside the scope of OZIPM.)

The rate constant for NO_2 photolysis and zenith angle is evaluated every hour using an algorithm developed by Schere and Demerjian (1977). The algorithm uses latitude, longitude, time zone, and date as input data to calculate photolytic constants. A set of third-order polynomial spline functions is then generated so that the photolytic constant for NO_2 and zenith angle can be easily calculated from a smooth curve for any time of the day. At a given zenith angle, all other photolysis constants used in OZIPM-3 are assumed to be either proportional to the NO_2 photolysis rate or a function of the zenith angle when specified explicitly by the user.

Emission rates are expressed either as fractions of the initial precursors or as emission densities for each hour. The emission rates are converted to continuous functions for use in solving the differential equations through a histogram-fitting algorithm described by Jeffries, Sexton, and Salmi (1981). The histogram-fitting algorithm replaced the spline-fitting algorithm described in the original OZIPP manual because the latter yielded widely oscillating functions.

Determination of Initial Concentrations

Before a simulation can begin, the concentrations of all pollutant species at the starting time must be determined by the program. These concentrations are derived from the initial concentrations of NMOC and NO_x that are specified by the User. The concentrations of transported pollutants are assumed to be zero unless otherwise specified by the INITIAL, TRANSPORT or BACKGROUND options (see Section 3).

The concentrations of the nonzero species are determined by the program in the following manner:

(1) NO_2 is set to the initial NO_x concentration multiplied by the NO_2/NO_x fraction (default is 0.25).

(2) NO is set to the initial NO_x concentration multiplied by the quantity one minus the NO_2/NO_x fraction.

(3) O_3 is set to the concentration transported in the surface layer or to the background value, whichever is larger (default is zero).

(4) The concentrations of the organic species are determined from the assumed initial NMOC concentration and the assumed reactivity fraction. Mathematically,

$$[\text{organic}]_i = [\text{NMOC}]\ (R_i)/C_i \tag{2-1}$$

where

$[\text{organic}]_i$ = i-th organic species in ppm

$[\text{NMOC}]$ = initial NMOC concentration, ppmC

R_i = carbon fraction of initial NMOC that is species i

C_i = number of carbon atoms in species i

Mathematical Formulation of Kinetics Model

The kinetics model in OZIPM mathematically simulates physical and chemical processes taking place in the atmosphere. This simulation is accomplished by numerically integrating a system of ordinary differential equations that describe the effects of these processes on pollutant concentrations. The result gives the concentration of pollutants as a function of time. The mathematical formulation of the system of differential equations is described next.

In OZIPM-3, five processes are assumed to affect pollutant concentrations:

(1) Chemical reactions
(2) Dilution
(3) Entrainment of pollutants transported aloft
(4) Emissions
(5) Surface deposition

Differential equations are used to describe the time rate of change of pollutant concentrations due to each process. The total time rate of change of each pollutant concentration is then simply equal to the sum of all these effects. Thus, the system of equations consists of one differential equation for each species in the kinetic mechanism. The five processes are described next.

Chemical Reaction Effects--

The change in pollutant concentration due to chemical reaction is a function of the rates of the chemical reactions. The rate of each reaction is the product of a rate constant and a concentration term. The photolytic rate constants are calculated by procedures that will be described later. The concentration term for unimolecular or pseudo-first-order reactions (such as photolytic reactions) is simply the concentration of the reactant. Bimolecular reaction rates are calculated similarly, except that the concentration term is the product of the two reactant concentrations. For example, the reaction rate (RT) for the reaction,

$$NO + O_3 \rightarrow NO_2 + O_2, \tag{2-2}$$

would be expressed as

$$(RT)_2 = k_2 \, C_{NO} \, C_{O_3}$$

where

$(RT)_2$ = rate of reaction 2, ppm min^{-1}

k_2 = rate constant for reaction 2

C_{NO} = concentration of NO, ppm

C_{O_3} = concentration of O_3, ppm

If the rate constant varies as a function of temperature, then k_2 would be represented by the rate constant at 298 K, along with an activation energy (E), in deg K, such that

$$k_2 \text{ (at temperature T)} = k_{298} \times \exp \left[E \left(\frac{1}{298} - \frac{1}{T}\right)\right] .$$

The time rate of change of a species due to chemical reaction is simply equal to the sum of all rates for those reactions in which the species is a product minus the sum of the rates for those reactions in which the species is a reactant. Thus,

$$\left(\frac{dC_i}{dt}\right)_R = \Sigma \, (RT)_{PROD} - \Sigma \, (RT)_{REAC} \tag{2-3}$$

$\left(\frac{dC_i}{dt}\right)_R$ = chemical reaction contribution to the time rate of change of species i

$\Sigma(RT)_{PROD}$ = the sum of all reaction rates in which species i appears as a product

$\Sigma(RT)_{REAC}$ = the sum of all reaction rates in which species i appears as a reactant

Dilution Effects--

The mathematical representation for simple dilution due to changes in the mixing depth is a first-order decay process. The rate of change due to this effect can be represented as follows:

$$\left(\frac{dC_i}{dt}\right)_D = -DC_i \tag{2-4}$$

where

$\left(\frac{dC_i}{dt}\right)_D$ = dilution effect contribution to the time rate of change of pollutant species i, ppm min^{-1}

D = dilution factor, min^{-1} (function of time)

C_i = concentration of species i, ppm

The dilution factor is calculated in one of two ways depending on the option chosen: The first method of dilution assumes that the mixing height varies from a minimum (or morning) mixing height to a maximum (afternoon) mixing height in accordance with a "characteristic curve" derived empirically from data taken during the St. Louis RAPS study (Schere and Demerjian, 1977). The "characteristic curve" represents the fractional growth in mixing height as a function of the fraction of daylight. The fraction of daylight is calculated as follows:

$$\text{Fraction of daylight} = \frac{\text{Time (current)} - \text{(time of sunrise)}}{\text{(time of sunset)} - \text{(time of sunrise)}}$$

The mixing height at any given time is

$$\text{Mixing height} = H_o + F_G \times \Delta H$$

where

H_o = mixing height at time of sunrise (calculated from the minimum mixing height)

ΔH = maximum mixing height - H_o

F_G = fraction of growth in mixing height.

The "characteristic curve" is depicted graphically in Figure 2. Note that before and after the inversion rise period, the dilution factor is zero since there are no dilution effects for those periods.

Two modifications were made to the characteristic curve concept to facilitate its use. First, a smooth curve through the points shown in Figure 2 was used to avoid discontinuities. Secondly, the mixing height at the start of the simulation (usually 0800 hours) was used instead of H_o as noted above since most simulations start after sunrise.

The second method of dilution is the specification of hourly mixing heights. When hourly mixing depths are specified, the dilution factor at each time step is calculated in the following manner:

$$D_t = \dot{H}T/HT_t$$

where

D_t = dilution factor at time t, min^{-1}

$\dot{H}T$ = the rate of change in mixing depth with time at time t, length min^{-1}

HT_t = mixing depth at time t, length.

Entrainment Effects--

Pollutants above the mixed layer are subject to entrainment. In OZIPM-3, these are limited to NMOC, NO_2, O_3, and up to 10 other chemical species. The mathematical treatment of entrainment assumes that the concentrations aloft do not change with time and that they extend uniformly to at least the height of the afternoon mixed layer. The pollutants entrained are assumed to mix rapidly within the enlarged surface layer. The mathematical expressions for the rates of change of the pollutants are shown by the following equations:

$$\left(\frac{dC_i}{dt}\right)_{AL} = D_t(C_i)_{AL} \qquad (2\text{-}5)$$

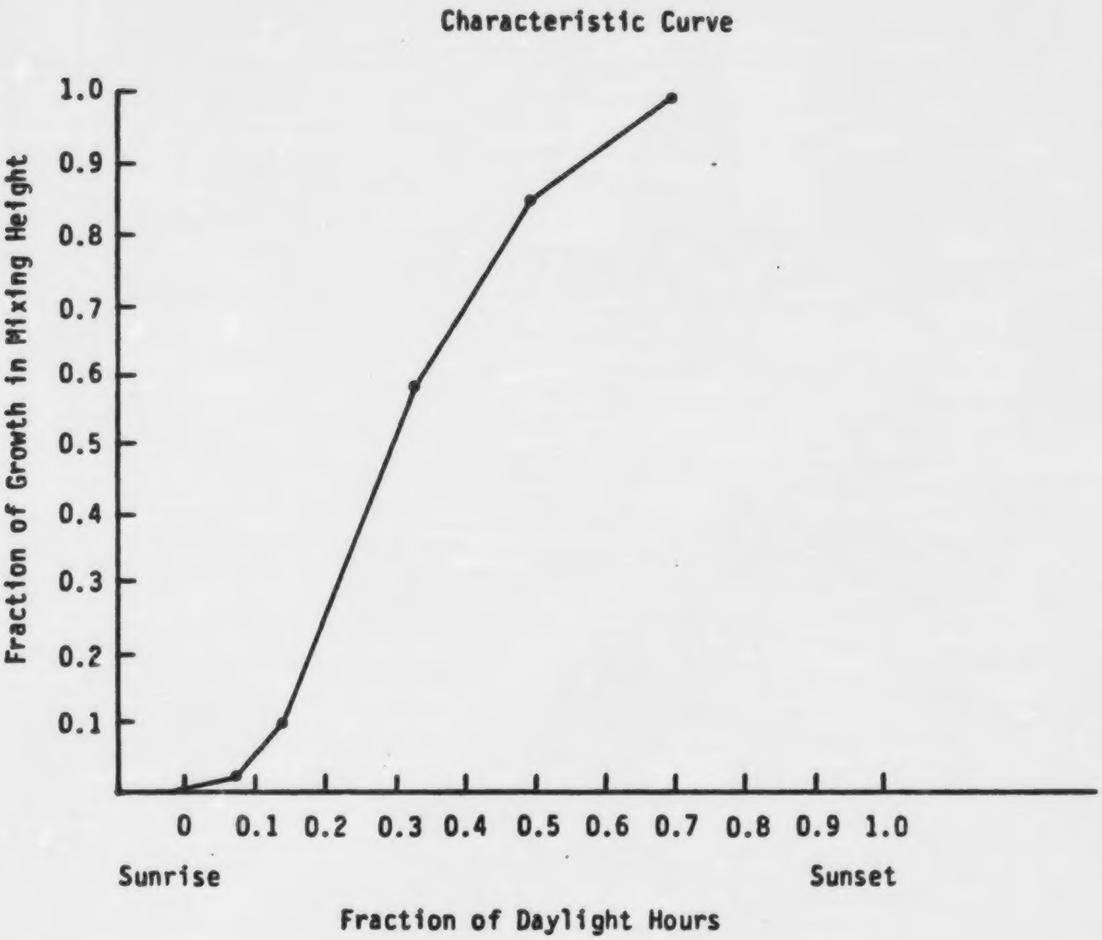

Figure 2. Graphical depiction of mixing height "characteristic curve."

$$\left(\frac{dC_{HC_j}}{dt}\right)_{AL} = D_t (C_{NMOC})_{AL}\ R_{HC_j}\ C_{HC_j} \quad , \qquad (2\text{-}6)$$

where

$\left(\frac{dC_i}{dt}\right)_{AL}$, $\left(\frac{dC_{HC_j}}{dt}\right)_{AL}$ = the contribution of entrainment to the time rates of change of species i or hydrocarbon species j, respectively, ppm min^{-1}

D_t = dilution factor (i.e., the rate constant at time t for the mixing height rise), min^{-1}

C_i = concentration of ozone, NO_2, and up to 10 other species trapped aloft, ppm

$(C_{NMOC})_{AL}$ = concentration of total nonmethane organic compounds trapped aloft, ppmC.

It should be noted that the effect of the change in mixing height is the sum of the dilution and the entrainment effects.

Emission Effects--

Emissions are the fourth factor affecting the rate of change of pollutant concentrations. The rates of change due to emissions are equal to the additional concentrations produced by the emissions. Because equal moles of emissions into different volumes will produce different concentrations, it is necessary to adjust the relative emissions to reflect the change in the column volumes due to the inversion rise. This is done internally in OZIPM by first calculating the ratio of the starting inversion height to the current inversion height. (This is equivalent to the ratio of initial volume to the current volume.) Before the inversion rise begins, this ratio is one. After the inversion rise has ceased, the ratio is the initial mixing height divided by the final mixing height. In general, the ratio (f_t) is the ratio of the initial mixing height to the mixing height at time t.

The rates of change due to the emissions are calculated from the values of the emission rates (calculated using the interpolating functions described earlier), the f_t ratio just described, and the reactivity inputs. The equations for the rates of change due to emissions for each of the affected species are shown below:

$$\left(\frac{dC_i}{dt}\right)_E = f_t(E_i)_t \quad ,$$

where

$\left(\frac{dC_i}{dt}\right)_E$ = emission contribution to the rates of change of species i, ppm min^{-1}

$(E_i)_t$ = value of emission rate, ppm per minute

For these formulations, a conversion from ppmC to ppm is performed for hydrocarbon species, and the reactivity of the hydrocarbons is taken into account.

The normal emissions input to OZIPM-3 is in fractions of initial NMOC and NO_x concentration, which gives ppm or ppmC emission rates. Other emissions options in OZIPM-3 allow the user to input mass or molar emissions rates. Molar emissions input to OZIPM-3 must be converted to normalized ppm units for the amount to be added each hour. The different emissions options available will automatically convert the emission density from moles $m^{-2}hr^{-1}$ to the required units; these options are discussed in Section 3. To convert emissions of moles $m^{-2}hr^{-1}$, one multiplies by 24450 moles^{-1} for each hour and divides by the initial mixing height m to normalize the values.

Surface Deposition Effects

The deposition rate is a function of surface type and the individual species' resistence to surface uptake. In general, NO, NO_2, and O_3 have high deposition rates, whereas organic compounds have very low deposition rates. Species surface deposition can be treated in a manner similar to that for dilution. In OZIPM-3 the rate of surface deposition is equal to the deposition velocity (in units of cm/s) times the pollutant concentration divided by the height of the mixed layer. Thus, the rate of change of the pollutants can be expressed as:

$$\left(\frac{dC_i}{dt}\right)_{\text{Deposition}} = - V_d \times C_i \div H \times 0.6$$

where V_d is the deposition velocity in units of cm/s, and H is the height of the mixed layer (m), and 0.6 is the conversion from cm/s to m/min.

Description of Numerical Integration

The kinetics model in OZIPM-3 employs a Gear-type integration scheme to numerically solve the set of differential equations described in the previous section. A detailed description is not given here because the method is not unique to OZIPM-3, and the procedure has been described elsewhere (Gear, 1971; Spellman and Hindmarsh, 1975; Sherman, 1975). The integration scheme initially uses a time step of 1×10^{-10} minutes (i.e., pollutant concentrations are to be calculated 1×10^{-10} minutes after the start time). Subsequent time step sizes are then computed by the Gear type integration scheme according to the estimated error at each step. The pollutant concentrations are calculated at each time step throughout the simulation period. (Once the final hour is reached, there is no restriction on precisely matching the final time step, since the concentrations can be interpolated back to exactly the last hour.) A typical simulation period takes from 150 to 200 time steps; about one-half of these time steps are used in simulating the first minute.

The total rate of change of any species is the sum of the rates of change due to dilution, entrainment, emissions, surface deposition, and chemical reaction just described. At each time step, the concentrations of all species are calculated along with the current rates of change for each species to predict the species concentration at the end of the time step using a Taylor-series type polynomial. The order of the polynomial is varied internally for optimum efficiency and is based on the values at the beginning of the time step. A corrective scheme then "corrects" the new concentration values, updates the Taylor polynomials, and estimates the average error. The corrector is a set of linear equations based on a Jacobian matrix whose elements are the set of partial derivatives of rate of change of concentrations of each species with respect to each of the other species. OZIPM-3 utilizes a linear system solving package for sparse matrices (i.e., those matrices in which most elements are equal to zero).

The integration method used in OZIPM-3 has been modified somewhat from the version published by Spellman and Hindmarsh (1975). For example, the error estimation is performed relative to the current concentration of a species rather than relative to its maximum concentration. The method utilizes the error estimate to determine the optimum step size and order, so that the allowable error specified by the user is met with the minimum number of integration steps.

The final task performed during the integration of the differential equations is determination of the maximum one-hour-average ozone concentration. Ozone concentrations are calculated for every minute of the simulation. This calculation is performed by interpolation between the actual time steps used in the integration. Running one-hour average concentrations are calculated using Simpson's rule and are updated every minute. The largest one-hour average concentration is then selected as the maximum.

SELECTION OF SIMULATIONS FOR GENERATION OF ISOPLETH DIAGRAMS

When generating an ozone isopleth diagram, the initial NMOC and NO_x concentrations for each simulation are selected internally by OZIPM-3. The program controls the selection of NMOC and NO_x concentrations so that maximum accuracy is obtained for the isopleth diagram from a given number of simulations. This is accomplished by

> Performing a minimum number of simulations for which the maximum one-hour-average ozone concentration is below the lowest isopleth line to be plotted.
>
> Minimizing the interpolation error between simulation points when constructing the ozone diagram.

Simulations are first performed at six individual points along the edges of the diagram. On the basis of the results of these simulations, additional simulations are then performed at points along lines of constant NMOC/NO_x ratio (i.e., a radial line emanating from the origin). The user can control the number of radial lines to be considered and the number of points on each radial line. Normally (i.e., under default conditions), similations are performed at five points along each of 11 radials. Finally, two more simulations are performed for individual points on the edges of the diagram to aid in plotting the lowest value isopleth. In all, 62 simulations are performed under default conditions.

Selection of Individual Points

The first step performed by OZIPM-3 in generating an isopleth diagram is to call for four simulations at NMOC and NO_x concentration corresponding to the four corners of the isopleth diagram as shown by points 1 through 4 in Figure 3. (Note that the user specifies the maximum NMOC and NO_x concentrations to be used). Next, two simulations (at points 5 and 6) are performed to estimate where the lowest value ozone isopleth will intersect the diagram edges. The concentrations for point 5 are determined using the maximum NO_x value and a NMOC value calculated by the following equation:

$$(C_{NMOC})_5 = \frac{(C_{O_3})_{LL} - (C_{O_3})_2}{(C_{O_3})_3 - (C_{O_3})_2} (C_{NMOC})_{MAX} \qquad (2\text{-}7)$$

where

$(C_{NMOC})_5$ = NMOC concentration at point 5

$(C_{O_3})_2$ = O_3 concentration at point 2

$(C_{O_3})_3$ = O_3 concentration at point 3

$(C_{O_3})_{LL}$ = The lowest ozone value to be plotted as an isopleth

$(C_{NMOC})_{MAX}$ = Maximum NMOC concentration on the diagram

Thus the coordinates of point 5 are calculated according to the assumption that at constant NO_x concentration, the maximum one-hour average ozone concentration is proportional to the NMOC concentration. This assumption of linearity is generally not true, but the results are used in the next-to-last simulation to calculate a more accurate location. An analogous procedure is performed for the right side of the diagram.

Selection of Radials and Points along Radials

After the simulations are completed for points 1-6, the program performs simulations at various points along selected radial lines (i.e., lines of constant $NMOC/NO_x$ ratio). The radial lines are used for the following reasons:

> Because most isopleths are roughly L-shaped, simulations at points on radial lines provide the highest density of simulation results near the region of highest curvature.
>
> Simplified theoretical considerations and empirical evidence show that along any radial line, it is easy to interpolate the maximum one-hour-average ozone concentrations as a function of distance from the origin of the isopleth diagram. Typically, these functions are

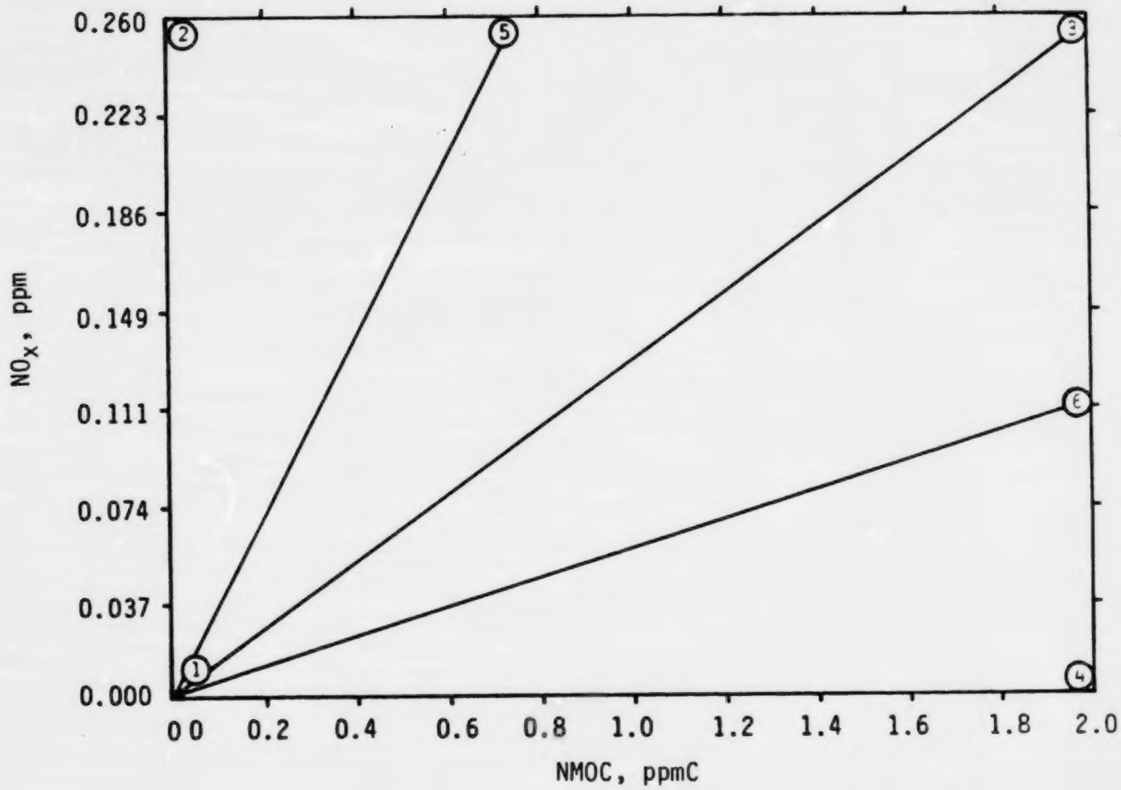

FIGURE 3. Initial simulation points.

nearly linear at low-to-intermediate ozone concentrations (e.g., 0.04 to 0.2 ppm ozone) and second order at high concentrations (> 0.5 ppm ozone). At the very lowest concentrations, various effects can lead to nonlinear behavior, but the functions needed to interpolate along the main part of the radial lines have few inflection points and therefore the interpolations should have a high degree of accuracy.

The first NMOC/NO_x ratio for a radial line corresponds to the diagonal line from the origin of the diagram to the opposite corner (i.e.,the point of maximum NMOC and NO_x concentrations). Simulations are then performed at various points along that diagonal (the user controls the number of points). The points on the radial are determined by estimating the locations of ozone concentrations along the line. The procedure begins with finding the ozone concentrations that form a geometric progression from the lowest ozone concentration to be plotted (e.g., 0.08 ppm) to the maximum ozone concentration at the terminal point of the radial. A geometric progression give the minimum relative change in ozone concentration from one point to another. The algorithm is built on the general assumption that the accuracy of the interpolation will be optimized if the relative change in ozone concentration between interpolation points is minimized.

To illustrate the procedure, assume that five simulations are to be performed along the diagonal radial. (Recall that the user can change the actual number of simulation points along the radial). Further, assume that the lowest ozone isopleth to be plotted is 0.08 ppm and that the values of NMOC, NO_x, and ozone at the terminal point of the radial are 2.0, 0.28, and 0.449 ppm, respectively. In general, the expression for the nth term of a geometric progression is

$$a_n = a_1 r^{n-1} \tag{2-8}$$

where

a_1 = the first term

r = the common factor

n = the number of terms

For the example problem, the geometric progression would be

0.08, 0.12, 0.19, 0.29, 0.449.

The common factor (r) was calculated as shown:

$$r = (0.449/0.08)^{1/4} = 1.54.$$

After determining the progression, the next step in the procedure is to estimate the NMOC and NO_x concentrations corresponding to the second highest ozone concentration in the progression (i.e., the first point along the radial below the terminal point). Linear interpolation is used in the following equation to estimate the NMOC value associated with this point.

$$(C_{NMOC})_P = (C_{NMOC})_{MAX} \frac{(C_{O_3})_P - (C_{O_3})_1}{(C_{O_3})_{MAX} - (C_{O_3})_1} \qquad (2\text{-}9)$$

where

$(C_{NMOC})_P$ = the NMOC value associated with the point

$(C_{O_3})_P$ = the projected ozone concentration associated with the point

$(C_{O_3})_{MAX}$ = the highest ozone concentration in the progression

$(C_{O_3})_1$ = the ozone concentration at point 1

For the example, the NMOC value corresponding to the projected 0.29 ppm ozone concentration is 1.30. Because the NMOC/NO_x ratio is constant at 7.14 along the line, the associated NO_x concentration is 0.18. Thus, a simulation is performed with NMOC and NO_x concentrations of 1.30 and 0.18, respectively.

The procedure for determining the locations of subsequent points along the radial is slightly different from the one just described. First, the original geometric progression is updated using the latest actual simulation result. In the example, the simulation result for the projected 0.29 point was actually 0.34 ppm, so the new progression becomes

0.08, 0.13, 0.21, 0.34,

with a new constant factor equal to 1.62. The problem is now one of estimating the location of the 0.21 ozone concentration on the radial. Once again, Equation 2-9 is used to predict the NMOC concentration associated with the projected 0.21 ozone concentration. However, because two interpolations fairly near each other have been completed (i.e., those giving ozone concentrations of 0.449 and 0.34, a linear extrapolation using these two points is performed to obtain a second estimate. These two estimates are then averaged to obtain the final NMOC value for simulation. This procedure (i.e., new progression, estimation by linear interpolation, estimation by extrapolation, and averaging of the two estimations) is repeated for each point except the last (i.e., the 0.08 point in the example). For this final estimation, a hyperbolic spline interpolation algorithm is employed.

Once all the simulations have been performed for all points on a radial, a new radial is chosen and the procedure is repeated. New radials are selected by estimating the location of the terminal points along the top or right edge of the diagram. The scheme for locating the terminal points is essentially identical to the one used in determining the points along the radial. An even distribution of the radial lines is important for obtaining accurate isopleth diagrams. Points too close to each other can introduce erroneous, high-frequency oscillations in the spline interpolations because of errors in the integration scheme. Points too far apart on the isopleth diagram itself leave large areas on the diagram in which no simulations have been performed. The initial concentration subsection contains internal tests for the termination points of the radial lines to avoid these difficulties.

INTERPOLATION AND PLOTTING OF ISOPLETH DIAGRAM

The interpolation and plotting section directs the construction of the ozone isopleth diagram using the results of previous simulations. Interpolation is done with hyperbolic splines rather than with classical polynomial types, because kinetic systems lead to curves resembling exponential functions. A noteworthy feature of the spline functions employed in this algorithm is the tension factor (Cline, 1974). The highest tension produces straight lines between points, whereas the lowest value produces roughly cubic fits.

Two stages of interpolation are used to generate the isopleths. In the first stage, the NMOC and NO_x coordinates of the ozone levels to be plotted are determined along each of the radials described in the preceeding section. The second stage draws a smooth curve for each ozone level through the points determined in the first stage. The curves are then plotted using the line printer and, if desired, an off-line plotter such as CALCOMP.

SECTION 3

DESCRIPTION OF OZIPM-3 OPTIONS

This section describes in detail the different options and card inputs available for use with the OZIPM-3 computer code. Currently, there are 25 options:

Optional Mechanism Input

MECHANISM - input chemical kinetic mechanism

ZENITH - input zenith angle dependence of the photolytic rate constants for optional mechanism or revise zenith angle dependence for the default mechanism

City-Specific Inputs

PLACE - location of the site

DILUTION - input minimum and maximum inversion heights

MIXING - input hourly inversion heights

TEMPERATURE - input hourly temperature values

DEPOSITION - input hourly surface deposition rates for specified species

TRANSPORT - input surface layer and aloft conditions of NMOC, NO_x, and O_3

INITIAL - input conditions of species transported in the surface layer other than NMOC, NO_x, and O_3; a simulation can be continued or restarted

ALOFT - input aloft conditions of species other than NMOC, NO_x, and O_3

BACKGROUND - input background conditions of NMOC, NO_x, and O_3

EMISSIONS - input hourly emission fractions of VOC and NO_x

MASSEMISS - input hourly mass emission densities of VOC and NO_x

MOLEMISS - input hourly molar emission densities of up to 5 species

REACTIVITY - input reactivity of the initial NMOC mix and VOC emissions and the initial NO_2/NO_x ratio

Additional Simulation Options

TITLE - input simulation title

TIME - input starting and ending times for computer simulations

RATE - change chemical reaction rate constants (for testing purposes)

SPECIES - input the species of interest for isopleths

ACCURACY - change the accuracy of the simulation (error tolerance) and the tolerance for spline interpolation

ALREADY - time saving option utilizing simulations from a previous run

PLOT - do off-line plotting (CALCOMP)

Program Output Options

EKMA - perform Level III procedures to obtain required VOC reduction

CALCULATION - do a single point on the isopleth

ISOPLETH - do the whole isopleth

The first four letters of each option have been underlined to denote the required input code.

Many of these options have been described in detail in the OZIPP user's manual (Whitten and Hogo, 1978a). The reader is referred to that document for detailed discussions of the following options: TITLE, PLACE, PLOT, CALCULATION, and ISOPLETH. These options are only discussed briefly here.

CHEMICAL KINETIC MECHANISM

The OZIPM-3 program has the capability to accept a chemical mechanism other than the default CBM-X that is internally stored in the program. The selected kinetic mechanism cannot contain more than 200 reactions and/or 90 species. For the computer program to handle different kinetic mechanisms, the user must input certain parameters:

> The total number of photolysis reactions (maximum of 20) and the reaction numbers that identify the photolysis reactions in the mechanism.
>
> The total number of organic species included in the initial NMOC mix (maximum of 15), the names that identify these species, and the number of carbon atoms in each.
>
> The fraction of total organic of each organic species listed above.

The following subsection discusses how mechanisms are coded into OZIPM-3.

Input of an Optional Mechanism

An optional mechanism is processed with the MECHANISM option code. On the MECHANISM card are entered the reaction identification number of the last reaction card of the mechanism to be entered, the total number of photolysis reactions, the total number of organic species in the initial mix, the mechanism input format, and the temperature. The program will then read the following card(s) in the following order:

> The list of photolysis reactions (up to seven on a card, twenty reactions maximum).
>
> The list of names for the organic species that are included in the initial NMOC mix (up to seven on a card, fifteen species maximum).
>
> The list of carbon numbers for the organic species in the same order as above.

After the list of carbon numbers for the species is read, the mechanism itself is input. For each reaction, a separate data card is used. Note that the species names used in the kinetic mechanism must be consistent (e.g., HO and OH will represent different species).

There are currently two input formats for the chemical reactions. The first format is similar to the formatting used in the chemical kinetics program (CHEMK) developed for the EPA (Whitten and Hogo, 1980). This format is provided for users who have chemical mechanisms setup for the CHEMK program. The CHEMK format allows for up to 3 reactants and 4 products per input card. Stoichiometric coefficients of one are assumed. As an example, the reaction $2NO + O_2 \rightarrow 2NO_2$ must be written in the following form: $NO + NO + O_2 \rightarrow NO_2 + NO_2$.

Since the stoichiometric coefficients for all reactants and products in each reaction are ignored in the CHEMK format, the user will need to rewrite certain reactions when using this format. The following reaction provides an example:

$$RCHO + h\nu \rightarrow 0.5\ RO_2 + 1.5\ HO_2 \qquad k_3 = 0.0025\ \mathrm{min}^{-1} \tag{3-3}$$

This reaction must be written so that all stoichiometric coefficients are equal to one. This can be done by separating the reaction into several reactions such that the sum of the new reactions will be equal to the original reaction (3-3).

In general,

$$A + B + C \rightarrow X_1D + X_2E + X_3F + X_4G \qquad k_4 \tag{3-4}$$

where the Xs are fixed such that

$$0 < X_1 < X_2 < X_3 < X_4 < 1.0 \ .$$

For the example case [Reaction (3-3)]

$$RCHO + h\nu \rightarrow 0.5\ RO_2 + 0.5\ HO_2 + 1.0\ HO_2 \tag{3-3}$$

the general Reaction (3-4) is written as four reactions:

$$A + B + C \rightarrow D + E + F \qquad k_5 \tag{3-5}$$

$$A + B + C \rightarrow E + F \qquad k_6 \tag{3-6}$$

$$A + B + C \rightarrow F \qquad k_7 \tag{3-7}$$

$$A + B + C \rightarrow \qquad k_8 \tag{3-8}$$

The rate constants for Reactions (3-5) through (3-8) are defined as follows:

$$k_5 = X_1 k_4$$

$$k_6 = (X_2 - X_1)k_4$$

$$k_7 = (X_3 - X_2)k_4$$

$$k_8 = (1 - X_3)k_4$$

Using this scheme for the example Reaction (3-3), the four reactions are

$$\mathrm{RCHO} + h\nu \rightarrow \mathrm{RO_2} + \mathrm{HO_2} + \mathrm{HO_2} \qquad k_9 \tag{3-9}$$

$$\mathrm{RCHO} + h\nu \rightarrow \mathrm{HO_2} + \mathrm{HO_2} \qquad k_{10} \tag{3-10}$$

$$\mathrm{RCHO} + h\nu \rightarrow \mathrm{HO_2} \qquad k_{11} \tag{3-11}$$

$$\mathrm{RCHO} + h\nu \rightarrow \qquad k_{12} \tag{3-12}$$

Rate constants for these reactions are

$$k_9 = 0.5k_{3'}$$

$$k_{10} = (0.5 - 0.5)k_{3'} = 0$$

$$k_{11} = (1.0 - 0.5)k_{3'} = 0.5k_{3'}$$

$$k_{12} = (1.0 - 1.0)k_{3'} = 0$$

Therefore, only Reactions (3-9) and (3-11) are needed to represent Reaction (3-3). Note that the sum of Reactions (3-9) and (3-11) is

$$\mathrm{RCHO} + h\nu \rightarrow \mathrm{RO_2} + \mathrm{HO_2} + \mathrm{HO_2} \tag{3-9}$$

$$\begin{array}{l} \mathrm{RCHO} + h\nu \rightarrow \mathrm{HO_2} \\ \hline 2\mathrm{RCHO} + 2h\nu \rightarrow \mathrm{RO_2} + 3\mathrm{HO_2} \end{array} \tag{3-11}$$

which is the same as Reaction (3-3). The general scheme outlined here applies to all reactions that can be transformed into the form of Reaction (3-4).

Each reaction card contains the reaction identification number, up to three reactants, up to four products, the rate constant at 298 K, and the activation energy in degrees Kelvin.

The second format for the chemical reactions allows the user to input nonunity stoichiometric coefficients for the products of the reaction. This format is an extension of the chemical mechanism input format for the EPASIM chemical kinetics computer program (Overton, 1976). The second format also allows the user to input up to nine products. For example the reaction

$$\mathrm{EL + NO \rightarrow 3\ NO_2 - 2\ NO + 0.5\ HO2 + 0.5(CHO)2 + 0.5\ CH_3CO_3}$$
$$\mathrm{+\ 0.5\ CH_3COCHO + 0.5\ CO}$$

can be input as follows:

(1) $\mathrm{EL + NO \rightarrow 3\ NO_2 - 2\ NO + 0.5\ HO_2}$

(2) $\mathrm{+\ 0.5\ CHO2 + 0.5\ ETO3 + 0.5\ ALLE + 0.5\ CO}$

where the numbers on the left side represent the card input sequence. Note that four character symbols are used in place of the actual species symbols. Each chemical reaction card contains up to three reactants, the reaction identification number, up to three products (with the associated stoichiometric coefficient), the rate constant at 298 K, and the activation energy in degrees Kelvin. If the reaction contains more than three products, the extra products are input in a continuation card with a flag to denote the continuation sequence.

For both formats the last reaction card must have a reaction number corresponding to the number given on the MECHANISM card even though it may not be the highest reaction number in the mechanism. Rate constants must be in $\mathrm{min^{-1}}$ for unimolecular reaction, in $\mathrm{ppm^{-1}min^{-1}}$ for bimolecular reactions, and in $\mathrm{ppm^{-2}min^{-1}}$ for termolecular reactions. The units of the activation energy (if used) must be in degrees Kelvin (K).

Photolysis reactions can be treated in one of two ways when inputting an optional mechanism into OZIPM-3:

(1) The rate of photolysis for a particular species can be assumed to vary with zenith angle in a fashion similar to NO_2. The rate constant for photolysis in such a case would then be expressed as some constant multiple of the rate constant for photolysis of NO_2. The user would input this multiple in the rate constant

slot of the reaction card. For example, if it is assumed that the photolysis of HNO_2 proceeds at a rate equal to 0.18 times the rate of photolysis of NO_2, the user would input a value of 0.18 in the rate constant field of the reaction card for HNO_2 photolysis.

Photolytic rate constants for NO_2 as a function of zenith angle are stored internally in OZIPM-3. Normally, when inputting a mechanism, the user would place a value of 1.0 in the rate constant field of the reaction card for NO_2 photolysis. The user, however, has the option to change the photolysis rate for this species. For example, to perform simulations with a 10 percent increase in the overall rate of NO_2 photolysis, the user would input a value of 1.10 in the rate constant field of the NO_2 photolysis card.

(2) The rate of photolysis for a particular species can be assumed to vary with zenith angle in a fashion that is not similar to NO_2. In this case, the user normally would input a value of 1.0 in the location on the reaction card where the rate constant is usually placed. He would then use the ZENITH option to input as a function of zenith angle the photolysis ratios relative to NO_2 for the species of interest. The ZENITH option is discussed in detail later in this subsection.

Modification of Rate Constants

Changes to any rate constant in the kinetic mechanism are made with the RATE card. On this card, the number of reactions with rate constant changes is placed in Columns 11-20. If a nonzero number is entered in Columns 21-30, a special option is activated in which all rate constants are set to zero except the photolysis rate constants. This allows the user to test the emissions, photolysis constants, and dilution rates. The photolysis rate constants can be set to zero with a PLACE card using a location above the arctic circle, near the winter solstice.

If only certain rate constants are to be changed, the next cards contain first the vector of reaction numbers with rate constant changes and then the vector of new rate constants for those reactions. The first card after the RATE card contains the reaction numbers (each located in separate 10-column fields; up to seven reaction numbers may be placed on a card). The next card(s) contains the new rate constants placed in the same location as that of the corresponding reaction numbers in the previous card(s).

ZENITH Option

Immediately following the MECHANISM option cards, the ZENITH option is used to revise or input photolysis rates as a function of zenith angles. In addition to those for NO_2, photolysis values for the following reactions are stored in OZIPM-3:

$$O_3 + h\nu \rightarrow O(^1D)$$

$$FORM + h\nu \rightarrow 2HO_2 + CO$$

$$FORM + h\nu \rightarrow CO$$

$$ALD2 + h\nu \rightarrow MEO2 + HO_2 + CO$$

Photolysis rates for these reactions are stored internally because these rates are known to vary with zenith angle in a fashion that is different from that of NO_2. Consequently, it would not be accurate to treat the photolysis of these species by coding a constant multiple of the NO_2 photolysis rate on the reaction cards as is done for the other photolysis reactions.

When using the CBM-X mechanism, the ZENITH option can be used to modify the default values that are stored internally for O_3, FORM, and ALD2. It can also be used to consider the zenith angle dependency for other species that are presently assumed to photolyze in a manner similar to that of NO_2. The user would input his choice of the ratio to NO_2 photolysis for these reactions at zenith angles of 0, 10, 20, 30, 40, 50, 60, 70, 78, and 86 degrees. (The use of a ratio to NO_2 photolysis was chosen because many of the photolytic rate constants are reported as a ratio to NO_2 photolysis in the literature.) Table 9 (Section 5) shows the format for the ZENITH option.

The default photolysis values for NO_2 can also be modified using the ZENITH option. For example, if the user wishes to increase the photolysis rate of NO_2 by 10 percent at a zenith angle of 0 degrees only, the user would input a value of 1.1 in Columns 11-20 of ZENITH option card 2. A value of 1.0 would be entered in the subsequent fields of the option cards.

When the MECHANISM option is invoked, all photolysis reactions are assumed to vary as a function of zenith angle in a fashion similar to NO_2 photolysis. Thus, the ZENITH option must be used when an optional mechanism is input into OZIPM-3 if the photolysis reactions for species such as O_3, FORM, and ALD2 vary with zenith angle in a fashion that is different from the NO_2 photolysis.

When an optional chemical mechanism is used, the user must follow the procedures outlined here to ensure proper use of the photolysis reactions:

The NO_2 photolysis reaction must be defined as the first reaction in the reaction list.

All photolysis reactions will have an associated multiplication factor, which is input in the slot normally reserved for the rate constant on the individual reaction card.

The multiplication factor changes the magnitude of the photolysis rate and is input as a ratio to the NO_2 rate.

For those photolysis reactions that do not vary with zenith angle in a fashion similar to NO_2, the user must invoke the ZENITH option immediately after the MECHANISM option cards.

Only those reactions that do not vary with zenith angle similar to NO_2 need be entered with the ZENITH option.

SITE-SPECIFIC INFORMATION

Up to 14 options can be used to describe the initial and meteorological conditions for the computer simulations. These options are PLACE, MIXING, DILUTION, TEMPERATURE, TRANSPORT, INITIAL, BACKGROUND, ALOFT, DEPOSITION, and TIME. Three different options (EMISSIONS, MASSMOLE, and MOLEMISS) can be used to describe the emissions entering the air parcel during the simulation. The option REACTIVITY is used to specify site-specific information on the reactivity of the initial NMOC and NO_x ambient mix and the VOC and NO_x emissions.

Place and Date

In all OZIPM-3 runs, the rate constants of the photolysis reactions in the kinetic mechanism are varied in accordance with the diurnal change in sunlight intensity (or solar zenith angles) during the specified simulation period. This diurnal variation is calculated using a computer code written by Schere and Demerjian (1977) that is incorporated in OZIPM-3. The user can adjust the photolysis rate constants to the area of interest by changing the date or location, or both, from the default values of 21 June 1975 at Los Angeles, California. The option is activated by the code word PLACE. The first three numeric fields of the PLACE card (Columns 11 through 40) contain the latitude (decimal degrees north), longitude (decimal degrees west), and time zone (hours from Greenwich Mean Time). The next three fields are used to specify the year, month, and day in Columns 41-50, 51-60, and 61-70, respectively. An additional card may be required after the PLACE card. On this card, the name of the city of interest is entered between Columns 1 and 24. This card is necessary only if a nonzero value for the latitude or the longitude is entered on the PLACE card. Therefore, even if the default values of 34.058 and 118.250 are entered, a second card is required with the name of the place. Users interested in the default location need not specify the latitude and longitude.

The correct set of numerical time zones for the continental United States is as follows:

Numerical Time Zone	Common Name
5.0	Eastern Daylight Time
6.0	Central Daylight Time
7.0	Mountain Daylight Time
8.0	Pacific Daylight Time

To produce standard time simulations, even though the output will show daylight time units, a false time zone can be created by incrementing the numerical time zone by one unit (hour). Thus, Pacific Standard Time photolysis constants would be generated if a 9.0 were entered instead of the correct 8.0 time zone. The output should then show that solar noon occurs near 1200 hours when the printing of solar noon is activated.

Dilution Rate

Dilution in OZIPM-3 occurs as a result of the rise in the early morning inversion. Under default conditions, the inversion is assumed to rise from 510 meters to 630 meters over a 7-hour period starting at 0800 LDT using the characteristic curve.

City-specific values for determining the characteristic-curve dilution rate are entered using the word DILUTE. The values of the morning mixing height, afternoon mixing height, inversion rise starting time, and inversion rise stopping time are entered in the first four numeric fields of the DILUTE card (i.e., Columns 11-20, 21-30, 31-40, and 40-50, respectively). The starting and stopping time should be in 24-hour time format, LDT. For both default and specific conditions, dilution is assumed not to occur outside the starting and stopping times.

Input of Hourly Mixing Heights

The second form of treating dispersion in OZIPM-3 allows the user to input hourly inversion heights if such data are available or if the user does not want to use the characteristic curve to calculate the mixing height profile. The user declares this option (MIXING) and gives the number of hours dilution is to occur. The inversion heights are then entered for the initial height and for the end of each hour. Therefore, if there are n hours of dilution, n+1 inversion heights are entered. Dilution will always start at the beginning of a simulation (i.e., zero time). To have a zero dilution rate for a certain number of hours, the same inversion height should be given for those hours. Note that zero cannot be used as an inversion height. Up to 24 hours of dilution may occur (corresponding to 25 inversion heights). Any measure of length may be used to specify the mixing heights, but the unit of measure must be consistent for all values entered. The format for the MIXING option is given in Section 5.

Temperature

Another option found in OZIPM-3 is the variation in temperature during a simulation period. The chemical kinetic mechanism can be dependent on the variation of temperature in the manner described by Whitten, Killus, and Hogo (1980). As the temperature rises, the kinetic mechanism generally reacts more rapidly, leading to earlier formation of ozone during the simulation period and possibly higher amounts of ozone. Temperature values are input in a manner similar to that in the MIXING option (described earlier and in Section 5). All temperature values must be in units of degrees Kelvin. If the TEMPERATURE option is not used, the default value is 303°K.

Surface Deposition

A new feature of OZIPM-3 is the treatment of dry deposition of gaseous species such as ozone, nitrogen dioxide, and sulfur dioxide. Hourly deposition velocities (in units of cm/s) are input for each species of interest. The format for surface deposition option (DEPOSITION) is the number of species with nonzero deposition rates followed by a series of cards that contain the species name and the first six hours of surface deposition rates. Additional hourly deposition rates are placed on cards following the first six hours of deposition rates. The user is referred to Section 5 for the format of the DEPOSITION option.

Initial Conditions of Transported Species

Initial concentrations of transported species are considered through two options. The TRANSPORT option is used to input initial concentrations of O_3, NMOC, and NO_2 transported in the surface layer and entrained from aloft. If the user selects the CBM-X Mechanism, then the use of the TRANSPORT card is exactly the same as that discussed in the OZIPP user's manual. If the user selects a different mechanism or wants to change the makeup of NMOC from the default value, a negative number must be entered that has an absolute value equal to the number of organic species in the kinetic mechanism. Similarly, a negative number is entered if there are organics entrained from aloft. The ozone (surface and aloft) and NO_2 (surface and aloft) are input in the same manner as described in the OZIPP user's manual. Immediately following the TRANSPORT card, the initial NMOC concentration and the fraction of the total organic for each organic species are input if there is to be NMOC transported in the surface layer. Similarly, the concentration of NMOC aloft and the fraction of the total NMOC for each organic species are input. Note that the fractions for the organic species can be different in the two cases. As is the case with all uses of the organic species, the fractions must be placed in the same order as the original list of names for the organic species input under the mechanism option.

To input species transported in the surface (or mixed) layer other than NMOC, O_3, and NO_2, an INITIAL option card can be used. The number of transported species is placed on this card. The next card(s) contains a list of names of the species that are to have nonzero initial concentrations. (Up to 80 species may have nonzero initial concentrations.) The next card(s) contains the initial concentrations (ppm) of the species listed on the previous card(s). This INITIAL option is useful for continuing a calculation beyond the 24-hour limit of the model.

To consider entrainment of species other than NMOC, O_3, and NO_2, an ALOFT option card can be used. The number of species with nonzero concentrations is placed on this card. The next card(s) contains a list of names of the species that are to have nonzero concentrations. (Up to 10 species may have nonzero initial concentrations.) The next card(s) contains concentrations (ppm) of the species listed on the previous card(s). These species will be entrained from aloft in a manner similar to that employed for ozone, NMOC, and NO_2, as previously described.

A set of background concentrations consisting of ozone, NMOC, and NO_2 can also be input by the user. The background concentrations represent the lowest limits that can be set for the transport concentrations in the surface and aloft layers. Therefore, if the user specifies values for O_3, NMOC, or NO_2 on the TRANSPORT card lower than the background values, then the background values will be used. The format for the BACKGROUND option is similar to that for the TRANSPORT option except that only one set of values for O_3, NMOC, and NO_x is entered (see Section 5).

In general, the concentrations of species transported in the surface layer and aloft remain constant for any simulation on an isopleth diagram. The EKMA option is the only option which allows the user to modify transported surface and aloft conditions for future year calculations.

Simulation Starting and Ending Times

Optional starting and ending times can be entered with the TIME card. The starting and ending times (Local Daylight Time, based on the 24-hour clock) are placed in the second (Columns 11-20) and third (Columns 21-30) ten-column fields, respectively. Times may be entered to the nearest minute, but the time difference (stop minus start) must not exceed 24 hours. Both the starting and ending times are set back to default values when a zero value is entered for the ending time.

Starting and ending times can also extend beyond midnight into the next day; the user need only specify the times. Note that the maximum of 24 hours for a simulation is not confined to a 24-hour period from midnight (0000 hr) to 2400 hours.

Emissions

One of the more extensive modifications to the original OZIPP code is the EMISSIONS option. Besides the EMISSIONS option described in the original OZIPP program, two new options (MASSEMISS and MOLEMISS) are available in OZIPM-3. The MASSEMISS option described in the OZIPM-2 user's manual (Gipson, 1984) allows the user to input VOC and NO_x emissions in units of kg/km^2. The hourly emission densities are converted to fractions of initial concentrations within the program based on the initial NMOC and NO_x concentrations, and the initial mixing height (in meters). This procedure is described in the 1981 city-specific EKMA guidelines (EPA, 1981). The MOLEMISS option allows the user to input emissions of VOC, NO_x, and up to three other species (e.g., CO and SO_2). The units of the hourly emissions values are in either ppm (ppmC for VOC) or moles (moles as carbon for VOC)/unit area. If moles/hr are input, the user must also input the initial mixing height, the horizontal area and the initial NMOC and NO_x concentrations. The VOC and NO_x emissions will vary according to the initial NMOC and NO_x concentrations, whereas the emissions from the other species are constant with changes in initial NMOC and NO_x concentrations.

As mentioned, up to five species may be input with the MOLEMISS option. The input species must be in the chemical kinetic mechanism (except for NO_x and VOC); otherwise, an error message will be printed. The nitrogen oxides emissions are input with the symbol NOX. The computer automatically splits NO_x into NO and NO_2, with a fixed NO/NO_x ratio of 0.95. Similarly, VOC emissions are input with the symbol VOC. The computer code will split the VOC emissions on the basis of the fractions input on the REACTIVITY card. The format for the MOLEMISS option requires the number of hours in which there are emissions, followed by the number of emission species. If units of moles are used, then the initial mixing height, followed by the horizontal area, is also added to the option card. The next card(s) will be the name vector for the emission species, followed by the emission values (6 on the first card; 7 on the second card; etc.) (See Section 5 for a more detailed description).

Reactivity of Initial Mix and VOC Emissions

Organic reactivity and the initial NO_2/NO_x ratio for both the 0600-0900 ambient mix and the VOC and NO_x emissions are input with the REACTIVITY card. This option must be used if the MECHANISM option is activated. The following entries must be made on the REACTIVITY card:

The number of organic species

The NO_2/NO_x ratio

If the number of organic species is nonzero, the next card(s) contains the vector describing the fractions of the total organic (per carbon basis) that each organic species represents. The order must be the same as that for the name and carbon number vectors entered earlier. The sum of the organic fractions should normally be equal to one. Note that the carbon fractions and NO_2/NO_x ratio for both the initial mix and the subsequent emissions must be identical. The default values for the organic fractions are set to the values recommended in Section 5, and apply only to the default CBM-X mechanism.

OUTPUT OPTIONS

Output options are of two types:

(1) Perform a single simulation

(2) Estimate VOC control requirements

A single simulation is performed using the CALCULATE option. Two methods are available in OZIPM-3 for estimating VOC control requirements in compliance with the EPA guidelines (1981). The first method (ISOPLETH) requires the generation of at least one isopleth diagram in which all calculations are performed on the diagram. The second method (EKMA) is an automated version of the EPA guidelines that estimates the VOC control requirement based on inputs of design ozone and $NMOC/NO_x$ ratio into OZIPM. The first method has been described in detail by Whitten and Hogo (1978a) and Gipson (1984). The second method (implemented in OZIPM-2) is described by Gipson (1984). The EKMA option has been enhanced to handle the Appendix B guidelines (EPA, 1981) procedures regarding post-control levels of transported pollutants.

All three options are discussed in detail in the following section.

Performing a Single Simulation (CALC)

Individual simulations can be performed at specified initial NMOC and NO_x concentrations using the CALCULATE card. The first two numeric fields on the CALCULATE card (Columns 11-20 and 21-30) specify the desired 0600-0900 ambient NMOC and NO_x concentrations. The initial conditions and hourly ozone concentrations will be printed to show the change of ozone with time during the simulation. Any number entered in the third numeric field (Columns 31-40) will activate an information option that will print

The rate constants used in the kinetic mechanism,

The concentrations of all species in the kinetic mechanism,

The net rate of change of all species,

The reaction rates for each reaction, and

The photolysis constants for all photolysis reactions.

If the information option is activated, the user can then specify the simulation time (in minutes) for which concentrations of all species, current reaction rates, etc., will be printed. The number of minutes after the simulation starting time at which the initial printing is made (default value = 60 minutes after start) is entered in Columns 41-50. The integral time step for which subsequent printings are made (default value = 60 minutes) is entered in Columns 51-60. Under default values, hourly concentrations of species, net rates of change, etc., are printed. After the simulation has ended, a concentration versus time profile is printed for ozone. An example of output from this option is given in Section 6.

Calculating VOC Control Requirements for a Specific Case (EKMA)

A feature added to the OZIPM-3 program is the ability to perform a VOC emission reduction calculation without generating an ozone isopleth diagram. When the EKMA option is used, the user must supply information on the design ozone level to be reduced, the NMOC/NO_x ratio to be used in the calculation, and the percent change in NO_x emissions. The calculations are performed in accordance with the procedures used to calculate control estimates from an ozone isopleth diagram (EPA, 1981) Through an iterative search procedure, the design point is first located by finding the initial NMOC and NO_x concentrations (in the specified ratio) that produce the desired ozone concentration (within 0.0005 ppm). A post-control point is then found by first adjusting the base-case NO_x point to reflect the change in NO_x emissions input by the user, and then finding the initial NMOC concentration that, along with the adjusted NO_x concentration, will produce an ozone value of 0.12 ppm (again, within 0.0005 ppm). The VOC reduction estimate is then calculated as the percent change in NMOC concentration from the base-case point to the post-control point.

Following Gipson (1984), the EKMA option is activated by an input record with the code word EKMA located in Columns 1-4. The design ozone value is then placed in the first numeric field of the EKMA input record. The second numeric field of this record contains the NMOC/NO_x ratio. The percent change in NO_x emissions that is expected between the base case and the post-control time periods is coded in the third numeric field. This value should be entered as the percent change. Thus, a positive entry corresponds to an increase, and a negative entry, to a decrease. (For example, a 5 percent increase would be coded as 5.0, and a 5 percent decrease, as -5.0.) The fourth numeric field is used to signify a change in transport conditions. If the same transport conditions are assumed for the base case and post-control case, this entry may be left blank. Otherwise, a numeric entry (e.g., 1.0) denotes that transport conditions to be used for the post-control case are different from those used for the base case, and these new values are coded in the next input record.

The first two fields of this next input record contain the surface and aloft ozone concentrations (in ppm), respectively. If a negative value is input, then future-year ozone transport is estimated using the curves described in EPA (1981) and shown in Figure 4. The third field contains the concentration of NMOC transported in the surface layer for the post-control situation. A negative value represents the median NMOC contribution factor as described in Appendix B of the 1981 guidelines. The fourth field represents the concentration of NMOC transported aloft for post-control conditions. A negative value represents a 40 percent reduction in present-day NMOC aloft. The next two fields (five and six) contain the future NO_x surface and aloft transport levels (in ppm). The last field (seven) of this record allows the user to calculate peak O_3 for a given percent reduction in NMOC. The user should note that the structure of this input record is similar to that of the TRANSPORT input record, but if any entry is left blank, then the base-case transport level will be used for the post-control case. Also, no provisions are included for making any changes to the composition of NMOC used in the simulations (i.e., the same NMOC transport composition will be used for both base case and post-control point).

As just described, the EKMA option causes the program to compute the VOC reduction (in percent) needed to lower the base ozone to 0.12 ppm. One additional option is available to the user to generate supplemental information. An entry of 1.0 in the fifth numeric field of the EKMA card generates a tabular report showing the change in ozone as a function of percentage change in VOC. Predicted ozone corresponding to VOC reductions of 10 percent, 20 percent, 30 percent, ..., and 100 percent, respectively, are printed. If a value of 2.0 is coded instead, the predicted ozone concentrations will also be written to a user-defined file, which might be used for subsequent analysis or graphical display. One output record is written to the file for each EKMA option that is activated. The output format consists of 11 fields, each 5 columns wide. The first field (Columns 1-5) contains the base-case ozone value. The remaining 10 fields contain the ozone predictions corresponding to the VOC reductions of 10 percent, 20 percent, 30 percent, ... 100 percent, in that order.

Generating an Isopleth Diagram (ISOP)

Up to six options can be used when generating an isopleth diagram: ISOPLETH, TITLE, PLOT, SPECIES, ACCURACY, and ALREADY. These options are described next.

ISOPLETH Option

In all OZIPM-3 isopleth diagrams, the origin represents 0.0 initial 0600-0900 NMOC concentrations (ppmC) and 0.0 NO_x concentrations. The

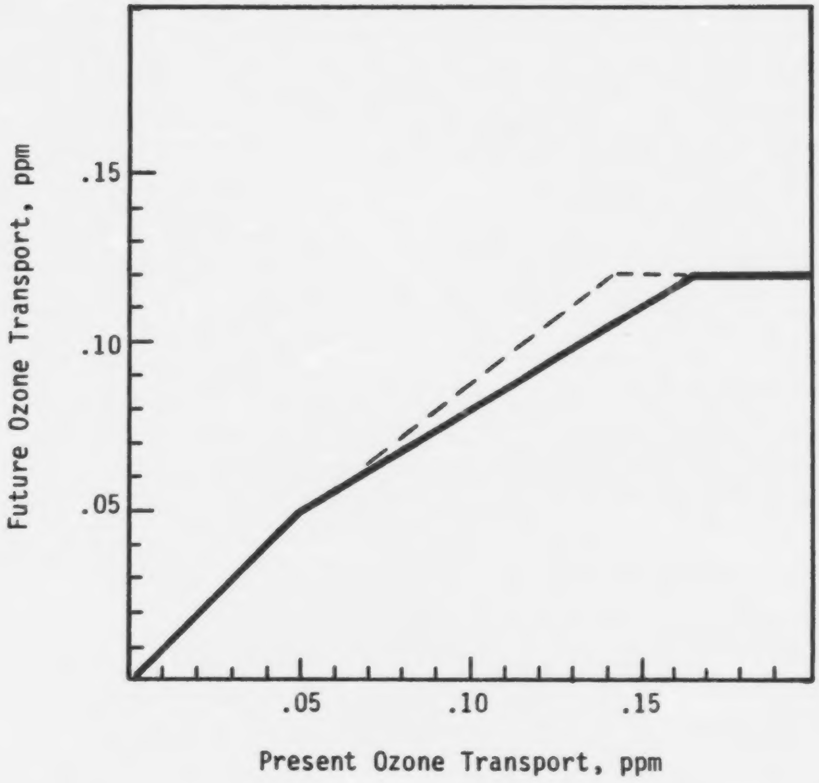

FIGURE 4. Future ozone transport as a function of present transport (source: EPA, 1981).

maximum NMOC and NO_x values represented on the abscissa and the ordinate can be changed from their respective default values of 2.0 ppmC NMOC and 0.28 ppm NO_x by putting the desired maxima into the first two numeric fields of the ISOPLETH card. The desired maximum NMOC concentration should be placed in the field of Columns 11 through 20. The desired maximum NO_x concentration should be placed in the field of Columns 21 through 30.

Any number can be used for the desired maximum NMOC and NO_x concentrations; however, because the scales on the abscissa and the ordinate are divided into ten and seven divisions, respectively, only certain values of the maxima will produce even markers. Thus, to produce an easy-to-use diagram, the NO_x maxima should be evenly divisible by seven (e.g., 0.14, 0.21, 0.28, 0.35, etc.). Similar consideration should be given to selecting an NMOC maximum.

The desired number of isopleths in the diagram should be inserted (followed by a decimal point) in the field of Columns 31 through 40 of the ISOPLETH card. Up to 20 isopleths can be drawn (the default value is 11). OZIPM-3 then reads the proper number of fields from the succeeding card or cards to provide the ozone concentrations (in units of ppm) for which isopleths are to be drawn. For example, inserting 10.0 in Columns 31-34 of ISOPLETH causes OZIPM-3 to read the seven 10-space numeric fields on the next card and three on the succeeding card. (As noted earlier, OZIPM-3 does not read past Column 70 on any card except the program title card.)

Currently, OZIPM-3 can only provide an isopleth for one species even though output results for more than one species are given when the SPECIES option is specified. Because the interpolation algorithms used to generate the diagram were optimized for typical ozone diagrams, isopleth diagrams generated for different species may not be produced correctly. Future revisions to the interpolation scheme and procedures for generating an isopleth diagram will be made so that diagrams can be generated for any species in one OZIPM-3 run. The user can generate a diagram for another species that has been declared with the SPECIES option by using the ALREADY option and placing the simulation results in the first column of the ALREADY option cards (see the section on ALREADY).

TITLE Option

The title can be changed by inserting a card with the word TITLE followed by a card with the desired title. Everything in Columns 1 through 72 of this title card will be printed on the output and isopleth diagrams in place of the default title, "Standard Ozone Isopleth Conditions." As with all options, these cards must precede the ISOPLETH or CALCULATE cards.

PLOT Option

Any plotting package that can be called using the standard CALCOMP subroutines can be used. Calls to these routines are activated by a card with the code word PLOT. This card must precede the ISOPLETH card. The actual CALCOMP routines called are PLOTS, PLOT, NUMBER, SYMBOL, and NEWPEN (if necessary). The use of the CALCOMP routines is discussed in Section 5.

The user also has the option to specify the actual size of the plot by defining the lengths (in inches) of the sides of the diagram. Columns 31-40 are used for the abscissa of the diagram. Columns 41-50 are used for the ordinate of the diagram. The size of title characters and axes numbers and the size of the isopleth labels can also be set by the user in Columns 51-60 and 61-70, respectively. The default values are given in Section 5. If the user wishes to reset any of these values, it is recommended that all values change proportionally.

Another option on the CALCOMP plots is the overlay of gridded lines on the isopleth diagram. This is done by declaring any nonzero positive values in Columns 21-30. If this option is exercised, a grid of different colors will be overlaid onto the diagram. If the user does not have access to the choice of different pen colors, use of this option is not recommended. If there is access to a matrix plotter (such as the VERSATEC plotter) and the choice of lines consists of thickness and pattern (i.e., dot-dash on solid patterns) the user can then enter a negative nonzero value in Columns 21-30. The absolute value of the number entered represents the user's choice of pattern and thickness. This number varies with different computer systems.

SPECIES Option

The OZIPM-3 package also has the capability of plotting an isopleth for any species in the kinetic mechanism. For instance, a user may be interested in plotting an NO_2 or PAN (peroxyacetylnitrate) isopleth. To activate this option, the user inputs a card with the word SPECIES in the first 10-column field and the number of species to be plotted. On the next card, the species names (or alphanumeric symbols), as used in the kinetic mechanism, are placed in the first four columns of each 10-column field (i.e., 1-4, 11-14, 21-24). The program will calculate maximum one-hour values for the species of interest. Isopleth diagrams will be generated for only the first species of interest when the ISOPLETH option is used, as noted earlier. If the SPECIES card is not used, the program will be set to the default species O_3 (ozone). The SPECIES option can also be used with the CALCULATE option to generate concentration-time plots for the species of interest.

ACCURACY Option

Most computing time for an OZIPM-3 run is expended in performing simulations. OZIPM-3 performs simulations at diagram points located along straight lines radiating from the origin of the isopleth diagram. In other words, OZIPM-3 performs several simulations on each of a number of lines of constant NMOC/NO_x ratio. The number of radial lines (i.e., lines of constant NMOC/NO_x ratio) and the number of simulations per line can be varied by the user. (OZIPM-3 also performs simulations at the corners of the isopleth diagram, and elsewhere, that cannot be controlled by the user).

Several options are available to OZIPM-3 users to allow reductions in computer costs. For example, using fewer radial lines in OZIPM-3 can produce an isopleth diagram at lower cost. However, the isopleths will have been interpolated from fewer points. For control strategy purposes, the default values of 11 radial lines and 5 simulations per line are recommended. Much computer time can be wasted through a poor choice of maximum NMOC and NO_x concentrations on the abscissa and ordinate of the isopleth diagram. When city-specific options are activated, some of the isopleth lines desired by the user may be off the diagram specified or may be cramped into a small part of the diagram. In addition, CALCOMP plotting may require extra time or added expense. In such cases, trial OZIPM runs without the CALCOMP option can be made with a reduced number of simulations. Then, the maximum NMOC and NO_x values that produce the best display of the ozone isopleth lines can be determined.

The number of radial lines used in the construction of the isopleth diagram can be controlled by specifying the desired number of lines (any odd number from 1 to 19) in the first numeric field (Columns 11-20) on the ACCURACY card. Leaving this field blank produces the default value of 11.

The number of simulations per radical line is controlled using the second field of the ACCURACY card (Columns 21-30). The possible values are 1 through 8 and the default value is 5. Thus, the isopleth diagram requiring the least computer time would result from a 1.0 in both of the first two numeric fields on the ACCURACY card. Essentially, only the diagram points at the corners of the diagram would be simulated. These results would be useful in estimating the VOC and NO_x factors that define the limits of an isopleth diagram.

ALREADY Option

Results from previous simulations can be utilized with the ALREADY card. To incorporate results from a previous run, the following conditions must be identical in both runs: the NMOC and NO_x scales, the city-specific options, the number of radial lines, and the number of simulations per line. Such a situation could occur when

An initial run is terminated because of a time restriction;

The user wishes to repeat the run with the PLOT option to obtain a CALCOMP-generated plot; or

The user wishes to alter the tension factors used in the interpolation schemes.

The user wishes to plot an isopleth for a species other than the first species specified by the SPECIES option.

To input the results of previous runs, the number of completed simulations is entered in the first numeric field (Columns 11-20) of the ALREADY card. The results of those simulations must be entered on the following cards in the same order in which they are calculated. Each card contains the results of one simulation. Field 1 (Columns 1-10) contains the initial NMOC concentration, Field 2 (Columns 11-20) contains the initial NO_x concentration, and Field 3 (Columns 21-30) contains the resulting maximum one-hour average O_3 (or other species) concentration. If a negative number of completed simulations is entered, then OZIPM will read the completed simulation results from an external file automatically generated by the OZIPM from the previous run.

A considerable amount of computer time is wasted when the maximum one-hour average O_3 concentration in a simulation occurs early but the simulation is continued for the full simulation period. The default condition in OZIPM forces this continuation because two ozone peaks often occur in simulations, and the second may be the larger. Nevertheless, a sizable reduction in computer costs is possible for simulations with single ozone peaks if the simulations are stopped after their peaks are reached. This can be done in OZIPM by placing any number in the sixth numeric field (Columns 61-70) of the ACCURACY card. However, the reasons for the occurrence of two ozone peaks are not well underdstood, so the full simulation period must be used to generate isopleth diagrams intended for control strategy use.

Multiple Isopleths

Any number of isopleth diagrams can be performed in one OZIPM-3 run. The user merely needs to insert the desired number of ISOPLETH cards. One set of simulations and an associated ozone isopleth diagram will be produced for each ISOPLETH card. Except for options that cannot be deactivated, all activated options will remain in effect until respecified and all input data will be fixed until redefined. Thus, if the default value for a parameter is desired in place of a value specified earlier, the default value must be respecified.

Once activated, the PLOT option and the first ozone peak option of ACCURACY cannot be turned off. If the ALREADY option has been activated, it will also remain activated until turned off (i.e., previous simulation results will be used with all subsequent ISOPLETH options). To deactivate the ALREADY option, another ALREADY card must be entered with a zero or blank in the first numeric field (Columns 11-20).

To illustrate the procedure for obtaining multiple diagrams, assume that the user wishes to produce two ozone isopleth diagrams, one to reflect default dilution conditions and the second to reflect different assumptions about dilution. The option cards might then be ordered as follows:

(1) A set of cards specifying all options and input values other than dilution (thereby invoking default dilution conditions).

(2) An ISOPLETH card resulting in production of an ozone isopleth diagram with default dilution condition.

(3) A DILUTION card specifying the new dilution condition.

(4) An ISOPLETH card resulting in production of an ozone isopleth diagram with the new dilution conditions.

Note that two sets of simulations are performed and that the same results may be obtained with two separate runs.

Testing the Accuracy of the Isopleth Diagram

Options have been incorporated into OZIPM-3 that allow users to test the accuracy of the diagram. In this manual, the term "accuracy" is always used in reference to the numerical solution of an implied initial value problem in ordinary differential equations. Thus, accuracy does not refer to the degree of correspondence between an isopleth diagram and atmospheric data.

Although the extensive experience gained in the development of OZIPM-3 suggests that the default radial lines, number of simulations per line, tension factor, and so on, will generate sufficiently accurate isopleth diagrams, this experience does not guarantee sufficient accuracy. Recommended procedures for checking many of the factors that affect accuracy are all similar. They merely answer the following question: Do somewhat higher or somewhat lower values of a particular factor significantly affect the resulting isopleth diagram? OZIPM-3 has been designed to respond properly to these factors. For instance, an increase in simulation density (more radial lines or more simulations per line) should produce a more accurate isopleth diagram. The procedures used in OZIPM-3 to check accuracy and to generate additional information are discussed next.

(1) Density of Simulations. As described earlier, the number of radial lines and the number of simulations per line can be decreased to reduce computer time by using the ACCURACY card. These numbers can also be increased to check accuracy. The first numeric field (Columns 11-20) of the ACCURACY card specifies the number of radial lines, and the second numeric field (Columns 21-30) specifics the number of simulations per radial line. The limits of acceptable input are odd numbers from 1 to 19 for the former and any number from 1 to 8 for the latter.

The accuracy of the points at which the isopleths touch the edges of the diagram can be checked (with minimal computer cost) by specifying 19 lines and 1 calculation per line. The accuracy of the isopleth lines along the diagonal of the isopleth diagrams can be checked by specifying 1 radial line and 8 simulations per line. The spacing and values along any one radial line can be checked by adjusting the diagram to make that line the diagonal (using the ISOPLETH card) and using the ACCURACY card with 1 radial line and 8 calculations on that line. (The ISOPLETH card must follow the ACCURACY card.)

(2) Accuracy of Simulations. The numerical integration scheme employed in OZIPM-3 estimates the degree of error at every step of the integration. The size of the time step taken by the computer is adjusted to keep the estimated error in the specified range. The error is conveniently controlled by a single parameter with a default value of

0.003. Smaller values of this parameter increase both the accuracy and computer time. Larger values do the opposite. By entering numbers smaller than 0.003 in the third numeric field of the ACCURACY card (Columns 31-40), one can estimate the accuracy of the simulations. For example, if several CALCULATE and ACCURACY cards are used, several simulations can be performed using the same NMOC and NO_x concentration, but using different time steps in the numerical integration. This procedure can be used to demonstrate how the simulation results vary with increased error tolerance.

(3) Spline Interpolation Accuracy. Unfortunately, the spline functions used to interpolate between simulation results do not have a parameter as relevant to accuracy as does the numerical integration scheme used for the simulations. The spline functions can be controlled to a limited extent by a simple factor that is analogous to tension. The lowest values for this factor (e.g., 0.001) cause the hyperbolic spline function to resemble cubic splines, whereas the high values (e.g., 50.0) result in virtually straight lines between points (or simply linear interpolation). Interpolation occurs in two different stages of OZIPM-3 and two factors are available to control tension. The first factor controls the first stage, namely interpolation between diagram points along the top edge of the isopleth diagram, along the right edge, and along each radial line. This interpolation stage estimates the coordinates of ozone concentrations for which isopleths are to be constructed.

The second factor controls the second stage of interpolation between diagram points calculated in the first stage to generate the coordinates of the isopleths themselves. Default values for both are 1.0, and the user can change these factors by entering the desired number in the fourth and/or fifth numeric field of the ACCURACY card (Columns 41-50 and 51-60). Thus, a value of 50.0 in the fourth numeric field of the ACCURACY card would cause nearly linear interpolation to be used to locate the diagram points on these radial lines and edges that correspond to the ozone concentrations at which isopleths are to be drawn. A value of 50.0 in the fifth field would result in nearly straight lines between diagram points calculated in the first stage.

To a limited extent, the tension factor for the first stage of interpolation controls the selection of NMOC and NO_x concentrations for some simulations because the same interpolation scheme is used in selecting the initial concentrations for the simulations. Therefore, using the results of a set of simulations (through the ALREADY option) with different first-stage tension factors may produce an isopleth diagram that is slightly different from one generated by recalculating the set of simulations.

SECTION 4

USING THE CBM-X IN OZIPM-3

The Carbon-Bond concept (Whitten, Hogo, and Killus, 1980) was developed mainly to simplify chemical kinetics mechanism use in atmospheric applications. Therefore, the simple procedures developed for earlier versions of the Carbon-Bond Mechanism used in EKMA and published in several documents can, for the most part, be applied to the use of the CBM-X. The most recent documentation for using Carbon-Bond chemistry in EKMA can be found in Killus and Whitten (1984) and Gipson (1984). The detailed development of the CBM-X is documented in Whitten, Killus, and Johnson (1985b).

The expanded version of the Carbon-Bond Mechanism (CBM-X) was developed specifically for use in atmospheric models such as EKMA, whereas previous versions of the CBM were designed to be used in complex photochemical dispersion models such as the Systems Applications' Urban Airshed Model (UAM) (see Reynolds et al., 1979). The size of these earlier versions was limited (i.e., number of reactions and species) to provide computational efficiency, whereas little effort was made to limit the size of the CBM-X since OZIPM-3 computer requirements are typically not large.

The expanded Carbon-Bond Mechanism (CBM-X) is actually a hybrid of explicit chemistry, surrogate approximations, and lumped/generalized chemistry designed to simulate the broad features of urban smog chemistry. Explicit chemistry is used to treat the inorganic and carbonyl species plus the chemistries of ethene, toluene, and xylene. Surrogate approximations are utilized by treating mono-substituted aromatics such as propylbenzene as toluene. The carbon-bond lumping method is used primarily for paraffins and olefins.

Each part of the CBM-X chemistry, such as the inorganic subset or the ethene chemistry, conforms to current literature review studies and has been extensively validated in separate organics/NO_x systems. In addition, the entire CBM-X was used to simulate a new series of auto exhaust and synthetic auto exhaust experiments involving a variety of conditions. Most of the smog chamber experiments used for CBM-X validation were performed in the outdoor dual-chamber facility of the University of North

Carolina, which is a well-characterized chamber with extensive analytical capabilities. The CBM-X also successfully simulated multiple-day experiments using a synthetic urban mixture of hydrocarbons performed in the outdoor dual smog chamber at the University of California at Riverside.

The main differences in the use of the CBM-X in OZIPM-3 compared to the use of CBM-3 involve the expanded carbonyl and aromatic chemistry. The new computer code also requires a different type of input for photolysis reactions, which vary differently from NO_2 photolysis as the zenith angle changes. These primary differences and some other minor ones are discussed in the following subsection. More detailed discussions concerning the conversion of atmospheric measurements and emissions profiles to carbon-bond species can be found in earlier documentation by Killus and Whitten (1984) and EPA (1984).

DEFAULT CBM-X MECHANISM

The default chemical mechanism implemented in OZIPM-3 is the CBM-X mechanism presented in Appendix A. The CBM-X mechanism consists of 67 chemical species and 148 chemical reactions. The CBM-X contains 8 primary organic species (see Table 1).

TABLE 1. CARBON NUMBERS OF CARBON-BOND GROUPS FOR PRIMARY SPECIES

Carbon-Bond Group	Carbon Number (carbon atoms per molecule)
PAR	1
ETH	2
OLE	2
TOL	7
XYL	8
FORM	1
ALD2	2 (acetaldehyde)
NR	1

The species NR represents the nonreactive part of different molecular species such as benzene, ethane, and acetylene. Several species whose concentrations do not vary (such as O_2 and N_2) are lumped in with the rate constant (for example, see Reaction 2 of Appendix A). In general, small changes in water concentration have little effect on the chemical mechanism. Hence, the concentration of water (H_2O) is lumped in with the rate constants (for example, see Reaction 17 of Appendix A). The concentration of H_2O used in the CBM-X corresponds to 50 percent relative humidity (20,000 ppm) at approximately 303 K. It is not recommended that this value be changed by the user.

The CBM-X mechanism shown in Appendix A is that discussed by Whitten, Killus, and Johnson (1985b) except that two reactions have been added. The first reaction,

$$OH \rightarrow HO_2 \quad k = 88 \text{ min}^{-1} \quad ,$$

is added to account for the natural background (see Killus and Whitten (1984) and EPA (1984) for further details). The second reaction,

$$NR \rightarrow NR \quad k = 1 \text{ min}^{-1} \quad ,$$

is added to account for the nonreactive species.

DEFAULT PHOTOLYSIS RATE CONSTANTS

The CBM-X chemical mechanism contains 18 photolysis reactions that vary with solar zenith angle. Thirteen of the photolysis reactions vary with zenith angle in a manner similar to that of NO_2 photolysis. Thus, the photolytic rate constants for these reactions can be described by applying a single multiplication factor to the NO_2 photolytic constant. The multiplication factor is input into the rate constant slot of the reaction card (see Section 5). Table 2 shows the multiplication factors used in the CBM-X mechanism for those reactions that vary in a manner similar to NO_2. Table 3 lists the default photolysis values for NO_2 that are stored in OZIPM-3.

Three species--O_3, FORM, and ALD2--photolyze as a function of zenith angle independent of NO_2 photolysis. The default ratios of these photolysis rates to NO_2 photolysis are shown in Table 4. Note that the multiplication factors for O_3, FORM, and ALD2 are nonunity in value. The values shown for these photolysis reactions represent an increase in overall photolysis to reflect the reaction rate constant at approximately 600 m above sea level. These photolysis rate constants are more representative of the entire mixed layer than they are of surface values. The user is able to change the default photolysis rate constants through the use of the ZENITH option.

TABLE 2. MULTIPLICATION FACTORS FOR CBM-X PHOTOLYSIS REACTIONS

Reaction Number	Reaction	Multiplication Factor
8	$O_3 + h\nu \rightarrow O(^1D)$	1.160
9	$O_3 + h\nu \rightarrow O(^3P)$	0.042
21	$HNO_2 + h\nu \rightarrow NO + OH$	0.18
26	$H_2O_2 + h\nu \rightarrow 2OH$	0.0014
30	$NO_3 + h\nu \rightarrow NO_2 + O$	26.0
31	$NO_3 + h\nu \rightarrow NO$	4.6
39	$FORM + h\nu \rightarrow HO_2 + HO_2 + CO$	1.1
40	$FORM + h\nu \rightarrow CO + H_2$	1.06
48	$ALD2 + h\nu \rightarrow MEO_2 + HO_2 + CO$	1.11
62	$MNIT + h\nu \rightarrow MEO + NO$	0.3
69	$AONE + h\nu \rightarrow MEO_2 + C_2O_3$	0.00004
72	$GLY + h\nu \rightarrow CO + CO$	0.0052
73	$GLY + h\nu \rightarrow CO + FORM$	0.0016
74	$GLY + h\nu \rightarrow 2HO_2 + 2CO$	0.0007
76	$MGLY + h\nu \rightarrow C_2O_3 + HO_2 + CO$	0.02
94	$KET + h\nu \rightarrow C_2O_3 + RO_2 + 2X$	0.0003
138	$BZA + h\nu \rightarrow PROD$	0.004

TABLE 3. NO_2 PHOTOLYSIS RATE CONSTANTS STORED IN OZIPM-3

Zenith Angle	Rate Constant*
0	6.00E-1
10	5.96E-1
20	5.85E-1
30	5.64E-1
40	5.31E-1
50	4.85E-1
60	4.09E-1
70	2.88E-1
78	1.55E-1
86	3.49E-2

* Units are min^{-1}.

TABLE 4. PHOTOLYSIS REACTION RATE RATIOS STORED IN THE OZIPM-3.*

Zenith Angle	ALD2 + hν → MEO2 + HO2 + CO	FORM + hν → CO	FORM + hν → 2HO2 + CO	$O_3 + h\nu \rightarrow O^{1D}$
0	6.44E-4	3.76E-3	2.71E-3	4.66E-3
10	6.24E-4	3.75E-3	2.70E-3	4.55E-3
20	6.05E-4	3.70E-3	2.61E-3	4.16E-3
30	5.40E-4	3.60E-3	2.48E-3	3.53E-3
40	4.73E-4	3.46E-3	2.28E-3	2.77E-3
50	3.74E-4	3.26E-3	2.01E-3	1.92E-3
60	2.74E-4	2.99E-3	1.64E-3	1.11E-3
70	1.91E-4	2.59E-3	1.25E-3	4.76E-4
78	1.08E-4	2.29E-3	9.15E-4	2.10E-4
86	5.40E-5	2.18E-3	6.90E-4	1.12E-4

* Ratios are relative to NO_2 photolysis. Rate constants are determined by multiplying the ratio by k_{NO_2}.

DEFAULT VOC AND NMOC REACTIVITIES

Since the organic species in the CBM-X mechanism (see Table 1) are the same as those found in the CBM-3 mechanism (Killus and Whitten, 1984; EPA, 1984), except that CARB (from the CBM-3) is divided into FORM and ALD2, and ARO (from the CBM-3) is divided into TOL and XYL, many of the procedures described by EPA (1984) for the use of the CBM-3 in EKMA apply to the CBM-X mechanism. Table 5 shows the recommended transported NMOC concentrations in the surface layer and aloft along with the default carbon fractions associated with the transported NMOC. Since OZIPM-3 does not contain any default concentrations for transported NMOC and aloft NMOC, it is recommended that the concentrations shown in Table 5 be used with CBM-X when no specific measurements are available. As discussed earlier, global background concentrations are represented by Reaction 147 in CBM-X. The NMOC values presented in Table 5 represent only the continental background. Table 6 contains a range of values that can be used for aloft NMOC concentrations. The highest concentrations represent "upset" conditions, which normally do not occur.

The procedures described by the EPA (1984) regarding the reactivities of the initial 0600-0900 NMOC mix and VOC emissions in the CBM-3 mechanism can also be applied to CBM-X. Table 7 contains the default reactivities for the 0600-0900 NMOC mix and VOC emissions. Note that there are two sets of values presented in Table 7. The first set represents a range of reactivities, and the second set represents specific values to be used in OZIPM-3 for CBM-X when no specific information is available. The range of reactivities was developed by Killus and Whitten (1984) on the basis of hydrocarbon measurements in several U.S. cities.

SELECTING A USER-SPECIFIED ORGANIC REACTIVITY

If 0600-0900 ambient organic measurements are available, they should be used to calculate organic reactivity rather than using the default carbon fractions that are stored in OZIPM-3. Table 8 shows how to determine the CBM-X fractions from 0600-0900 ambient data reported in moles/ℓ.

The following paragraphs describe step-by-step how the organic reactivity is defined based on the ambient measurements shown in Table 8. Before we discuss these procedures, we note that in general ambient measurements are reported in the following units:

TABLE 5. DEFAULT NMOC FRACTIONS USED IN OZIPM-3.

Species	Carbon Fraction Transported Surface Layer	Aloft Layer
ETH	0.05	0.06
OLE	0.03	0.03
ALD2	0.16	0.09
FORM	0.10	0.06
TOL	0.07	0.08
XYL	0.06	0.07
PAR	0.53	0.61
NR	0.00	0.00
Total NMOC (ppmC)	0.038	0.040

TABLE 6. REACTIVE ORGANICS ALOFT

Carbon Fraction		Total NMOC Concentration (ppmC)	Species
Low	0.91	0.033	PAR
	0.09		FORM
Mid*	0.61	0.058	PAR
	0.08		TOL
	0.06		ETH
	0.03		OLE
	0.06		FORM
	0.09		ALD2
	0.07		XYL
High	0.54	0.174	PAR
	0.04		TOL
	0.02		XYL
	0.11		ETH
	0.07		OLE
	0.11		FORM
	0.11		ALD2

* These are the default carbon fractions in OZIPM-3.

NOTE: All estimates include 0.015 ppmC PAR as surrogate for background methane.

TABLE 7. REACTIVITY OF INITIAL MIX AND VOC EMISSIONS

Bond Type	Carbon Fraction Range	Default Value
ETH	0.02 - 0.11	0.04
OLE	0.02 - 0.07	0.03
ALD2	0.02 - 0.07	0.03
FORM	0.01 - 0.03	0.02
TOL	0.05 - 0.25	0.12
XYL	0.03 - 0.20	0.10
PAR	0.4 - 0.70	0.51
NR	0.05 - 0.22	0.15

Example 2

TABLE 8. Carbon-bond splits for Los Angeles ambient measurements.*

(a) Carbon-Bond Group Concentrations

Compound	[RH],ppm Molar Basis	Number of Each Bond Group x Concentration							
		NR	OLE	ETH	PAR	FORM	ALD2	TOL	XYL
CH_4	2.01								
C_2H_6	0.049	0.078			0.0196				
C_2H_4	0.043			0.043					
C_2H_2	0.038	0.038			0.038				
C_3H_8	0.037	0.0555			0.0555				
C_3H_6	0.0087		0.0087		0.0087				
iso-C_4H_{10}	0.012				0.048				
n-C_4H_{10}	0.037				0.148				
1-C_4H_8	0.0015		0.0015		0.0030				
iso-C_4H_8	0.0030				0.009		0.003		
iso-C_5H_{12}	0.0443				0.2215				
n-C_5H_{12}	0.0162				0.0810				
Cyclo-C_5H_{10}	0.0026				0.013				
1-C_5H_{10}	0.004		0.004		0.012				
2-Methylbutene	0.0008				0.0008		0.0016		
2,3-Dimethylbutane**	0.0008				0.0048				
2-Methylpentane	0.0110				0.066				
3-Methylpentane	0.0100				0.06				
1-Hexene	0.0017		0.0017		0.0068				
n-Hexane	0.0100				0.06				
Cyclohexane***	0.0107				0.0642				
2,2,3-Trimethylbutane	0.0077				0.0539				
C_6H_6	0.0082	0.041			0.0082				
2-Methylhexane	0.0069				0.0483				
3-Methylhexane	0.0063				0.0441				

Continued

* Source of hydrocarbon data: Calvert (1976).

** Incorrectly reported as 2,2 dimethylbutene by Calvert (1976).

*** Incorrectly reported as cyclohexene by Calvert (1976).

TABLE 8. Concluded.

Compound	[RH],ppm Molar Basis	NR	OLE	ETH	PAR	FORM	ALD2	TOL	XYL
		Number of Each Bond Group x Concentration							
1-Heptene	0.0044		0.0044		0.022				
n-C_7H_{16}	0.0043				0.0301				
Methylcyclohexane	0.0037				0.0259				
2,2,3- and 2,3,3-Trimethylpentane	0.0019				0.0152				
2,2,4-Trimethylpentane	0.0025				0.02				
Toluene	0.020							0.02	
1-Methylcyclohexene	0.0047		0.0047		0.023				
2,2,5-Trimethylhexane	0.0010				0.009				
n-C_8H_{18}	0.0021				0.0168				
EtC_6H_5	0.0041				0.0041			0.0041	
p,m-Xylenes	0.014								0.014
o-Xylene	0.0060								0.006
n-C_9H_{20}	0.0013				0.0117				
n-PrC_6H_5	0.0010				0.002			0.001	
sec-BuC_6H_5	0.0050				0.015			0.005	
n-$C_{10}H_{22}$	0.0011				0.011				
n-$C_{11}H_{24}$	0.0010				0.011				
n-$C_{12}H_{26}$	0.0003				0.0036				
CO	1.91								
Total		0.2125	0.025	0.043	1.2944		0.0046	0.030	0.020

(b) Carbon-Bond Splits

Compound	NMHC (ppm)	ppmC	Carbon Fraction of NMHC	Adjusted Carbon Fraction*
NR	0.212	0.212	0.105	0.105
ETH	0.043	0.086	0.042	0.042
PAR	1.294	1.294	0.640	0.640
FORM				0.020
OLE	0.025	0.050	0.025	0.025
ALD2	0.0046	0.092	0.005	0.035
TOL	0.030	0.21	0.104	0.104
XYL	0.020	0.16	0.079	0.079

*Carbon fraction adjusted to account for the aldehydes that were not measured.

ppm (parts per million)
pphm (parts per hundred million)
ppb (parts per billion)
$\mu g/m^3$ (micrograms per cubic meter)

In some cases the organic compounds may be expressed in the above units either as a molecular total or as a carbon total (i.e., the actual moelcular weight or the molecular weight of carbon is used). In general, chemical mechanisms are based on molecular reactions or the number of molecules involved. The first three units presented above are in the units necessary for most chemical mechanisms. The fourth unit is a mass unit and must be converted to molecular units. The following equation is used to convert mass units to molecular units:

$$C_{ppm} = \frac{0.0244}{MW} \times C_{\mu g/m^3} \quad ,$$

where MW is the molecular weight in units of g/moles of the organic compound. Molecular weights for each compound are given in Table B-1. The conversion factor, 0.0244, is based on the perfect gas law at 25°C and standard pressure. To obtain molecular units as carbon, one needs to multiply by the number of carbons found in the organic compound.

Table 8 shows ambient organic compound measurements in the Los Angeles area (Calvert, 1976). The measurements are reported in molar units (ppm in this case); to obtain the carbon-bond reactivity, one must assign the individual carbon atoms of each organic compound to the appropriate carbon-bond group according to Table B-2 in Appendix B. Table B-2 shows the breakdown of each carbon atom from the molecular compound to the carbon-bond groups. For example, the organic compound C_3H_6 (propylene) shown in Table 8 comprises one OLE and one PAR. Thus, of the three carbon atoms of propylene, two are assigned to OLE (because each OLE group contains two carbons), and one is assigned to PAR. To calculate the concentrations of OLE and PAR from propylene, we multiply the number of each bond group by the concentration of propylene. Thus, the propylene concentration of 0.0087 ppm produces 0.0087 ppm of OLE and 0.0087 ppm of PAR. As another example, Appendix B shows that benzene (C_6H_6) consists of five NR and one PAR. Applying the above procedures, we obtain 0.041 ppm of NR and 0.0082 ppm PAR.

The above procedure is followed for all the organic compounds identified in Table 8. The carbon-bond concentrations are summed as shown in Table 8(b). The OZIPM-3 requires all organic fractions to be on a "per-carbon" basis. Thus, the concentrations for each carbon-bond group are multiplied by the appropriate number of carbons reported in Table 1 and normalized to obtain the carbon fractions, as shown in the fourth column of Table 8(b).

In the example presented in this section, only surrogate carbonyls could be included in the speciations because carbonyl compounds per se (aldehydes and ketones) could not be detected by the instrumentation used. Carbonyl compounds were undeniably present, however, and they are significant contributors to smog chemistry. Therefore, some estimates of carbonyl emissions must be made. Investigations by Killus and Whitten (1984) show that an estimated 5 percent of the total organics are carbonyls. Of the 5 percent, 60 percent is ALD2, and 40 percent is FORM. Thus, for those cases in which there are no measured carbonyls, we must add 5 percent carbonyls (3 percent ALD2 and 2 percent FORM) to the total organics. The carbon fractions adjusted for the carbonyls are shown in the fifth column of Table 8(b). The numbers shown in this column are input into the OZIPM-3 program.

SECTION 5

USER'S GUIDE

This chapter describes the format of the input data, the types of errors and warning messages that can occur, and some special problems to be considered in the installation of the program on a specific facility.

FORMAT OF INPUT DATA

The 25 options in OZIPM-3, which were discussed in Section 3, are listed in Table 9.* For each option, the locations of the different parameters on the appropriate cards or card images are shown. The order of the OZIPM options in the input deck is not important except for the ISOPLETH, EKMA, and CALCULATE options. Any options to be activated for simulations must precede these three options. Consequently, the order shown in Table 10 is recommended. This ordering has the MECHANISM and ZENITH options listed first, followed by the options used to input city-specific information (PLACE, DILUTION, EMISSIONS, REACTIVITY, TRANSPORT, etc.). The next group of options affects some of the operational aspects of OZIPM (ACCURACY, ALREADY, PLOT, SPECIES, and TIME). The options that actually initiate simulations follow (CALCULATE EKMA, and ISOPLETH). The last card of any input set must be a blank card.

As shown in Table 9, all four-letter code words (e.g., TITL, PLAC, etc.) that activate an option must begin in Column 1. Each card containing such a code word has up to six numeric fields, each ten spaces wide, beginning in Column 11. An entry can be made anywhere in a field, but a decimal point must always be used, even with integral values. Additional data cards are associated with some options. These cards must follow the option card in the order specified in Table 9. For example, the card containing the title must immediately follow the card with the code word TITL. Data cards that do not begin with code words can contain up to seven 10-column fields beginning in Column 1. Similar to the numeric fields on cards with code words, entries may be made anywhere in the field provided a decimal is used.

---

* For convenience, Table 9 appears at the end of this section.

As previously described, most parameters have associated default values. These are indicated by DF in Table 9. If no entry is made in a numeric field, the default value will be assumed. For example, if the only entry made on the PLACE card is in the first numeric field, the default value of 118.25 will be assumed for the second numeric field, 8.0 for the third, etc.

PROGRAM-GENERATED ERROR MESSAGES

This section discusses potential output error messages produced by OZIPM. Two types of error messages can be generated:

(1) Fatal error messages--messages caused by problems that immediately halt any further computation.

(2) Nonfatal error messages--messages caused by problems that do not cause an immediate halt in computation.

These types of messages are discussed next.

Fatal Error Messages

Seven fatal error messages can occur during OZIPM runs. Five of these occur because the integration scheme cannot proceed further. Descriptions of each message are included here:

THE LOWEST OZONE LINE CANNOT BE PLOTTED; INCREASE THE MAXIMUM HC AND NO_x VALUES

If the concentration of ozone predicted from the maximum NMOC and NO_x concentrations (listed on the ISOPLETH card, or NMOC = 2.0, NO_x = 0.28 by default) is less than the lowest ozone isopleth line to be plotted, the program will stop. The user can fix this problem either by increasing the maximum NMOC or NO_x concentrations or by reducing the concentrations at which ozone isopleths are to be plotted.

NO LINES CAN BE PLOTTED; BACKGROUND ONLY PRODUCES TOO MUCH OZONE ______ PPM

This message is the opposite of the previous message. If the amount of ozone predicted at NMOC and NO_x concentrations of 0.0 is greater than the highest ozone isopleth line desired, the program will stop.

The following error messages all stem from problems encountered in the integration scheme routines:

PROBLEM APPEARS UNSOLVABLE WITH GIVEN INPUT

INTEGRATION HALTED BY DRIVER AT T - ____, EPS TOO SMALL TO BE ATTAINED FOR THE MACHINE PRECISION

KFLAG = -2 FROM INTEGRATOR AT T = ______, H = ______ THE REQUESTED ERROR IS SMALLER THAN CAN BE HANDLED

KFLAG = -3 FROM INTEGRATOR AT T = _____ CORRECTOR CONVERGENCE COULD NOT BE ACHIEVED

ILLEGAL INPUT..EPS.LE.0

If any of these messages occur, the user should try the following procedures:

Check input to be sure all data are correct (e.g., check NMOC and NO_x values on a CALCULATE option, check for negative error tolerance, and so on).

Raise the value of the error tolerance, if necessary.

Redefine the density of simulations (e.g., change the number of radials, number of simulations per line, maximum NMOC or NO_x concentrations, etc.).

As a last resort, alter the simulation conditions slightly (e.g., change emissions, dilution, etc.).

Nonfatal Error Messages

Two nonfatal error messages can occur in OZIPM runs. The user may wish to redefine the situation (i.e., the limits of the diagram) or to check the input data.

THE OPTIONS INSTRUCTION___CANNOT BE PROCESSED

If this message occurs, the user should check for an error in the input data.

DUE TO HIGH BACKGROUND CONDITIONS THE LOWEST OZONE PLOTTED WILL BE ____PPM

This message indicates that some of the desired ozone isopleths lie outside the limits of the diagram. For example, if the maximum ozone concentration associated with zero emission factors were greater than 0.08 ppm, a 0.08 ppm isopleth could not be drawn. However, isopleths greater than 0.08 ppm could possibly be drawn.

COMPUTER CONSIDERATIONS

The OZIPM program consists of one main program and 55 subprograms. It requires about 30,000 16-BIT words of core in a PRIME 750 computer system. Run times on the system average 1 1/2 hours. Complete listings, along with flow diagrams of selected subroutines, are shown in Volume 2. Also included are five calls to CALCOMP subroutines. Following paragraphs discuss special language considerations, use of CALCOMP routines, and computer control language.

Language Considerations

Although OZIPM has been written to conform with ANSI standard FORTRAN language, certain aspects of usage in OZIPM are not compatible on all computer systems. The variable UROUND in subroutine DRIVES should be set to the round-off error associated with each computer system. Currently, UROUND is set to the round-off error of 2.4×10^{-7} associated with a PRIME 750 computer system. To reset UROUND, the card in the BLOCK DATA routine should be changed as follows:

```
DATA   UROUND/user's round-off error/
```

UROUND is calculated form the number of significant digits (N) used for the mantissa of a floating point constant:

$$\text{UROUND} = 2^{-N}.$$

For the PRIME 750 computer, each word contains 32 BITs, of which 22 are used for the mantissa. Thus, 2^{-22} is equal to approximately 2.4×10^{-7}. This is the value currently set in OZIPM.

Another variable in OZIPM that is machine-dependent is EXPMAX, which is found in subroutines CURV1 and KURV1. This variable represents the maximum possible value for the exponent of e. For the PRIME computer, the range of the real constants is from 10^{-38} to 10^{38}. Hence, the maximum value for the exponent of e is

$$e^{EXPMAX} = 10^{38},$$

i.e., EXPMAX is 87.4 for the PRIME computer, the value currently set in OZIPM-3. To reset EXPMAX, the user must change the cards accordingly:

```
        DATA EXPMAX/user's maximum exponent/        CURV1
and
        DATA EXPMAX/user's maximum exponent/        KURV1
```

Use of CALCOMP Routines

The CALCOMP routines required by OZIPM are

```
Subroutine PLOT (XX,YY,IX)
           PLOTS (XX,UU,IX)
           SYMBOL (XX,YY,HT,ITX,ANG,NCH)
           NUMBER (XX,YY,HT,FPN,ANG,NDEC)
           NEWPEN (IPEN)
```

For users without access to these CALCOMP routines, dummy routines may be needed to run OZIPM. To generate the dummy routines, the user must have the following cards for each of these CALCOMP routines:

```
SUBROUTINE________(argument list)
RETURN
END
```

For users with access to standard CALCOMP routines, no modifications to OZIPM are required. The user should check to ensure that the five routines in their system have the same names as those given above.

Control Language--

Since the job control language necessary to run OZIPM-3 is different for each computer system, only the files required by the program are discussed in this section. Table 10 lists the files and the FORTRAN file unit numbers used by OZIPM-3.

TABLE 9. INPUT FORMAT FOR OZIPM OPTIONS

Option	Card No.	Column	Contents
MECHANISM	A kinetic mechanism may be input with this option		
	1	1-4	MECH
		5-10	Not read
		11-20	The identification number on the last reaction card to be read in (MAX = 200) If a negative number is entered, then the default mechanism will be printed
		21-30	The number of photolysis reactions found in the mechanism (MAX is 20; DF = 18)
		31-40	Number of organic species in the 0600-0900 ambient mix (MAX = 15; DF = 8)
		41-50	Chemical reaction format (nonzero for CHEMK format; DF = nonunity stoichiometric coefficient format)
		51-60	The temperature (in degrees K) used for the simulations (DF = 303)
		61-80	Not read
	2	1-10 11-20 . . .	The list of reaction numbers identifying the photolysis reactions in the kinetic mechanism (up to seven on a card).
		61-70	Continue on next card (if necessary)
		71-80	Not read
	3	1-4	The list of names (or alphanumeric symbol) for the set of organic species Continue on next card (if necessary)
		61-64	
		65-68	Not read

TABLE 9 (continued)

Option	Card No.	Column	Contents
MECHANISM	4	1-10 . . . 61-70	The list of the number of carbons associated with each of the organic species. Must be in the same order as the organic species name vector on the previous card(s). Continue on next card (if necessary)
		71-80	Not read
	The mechanism is entered next.		
	There are two formats:		
	7+(CHEMK format)	1-3	The identification number of the reaction (right-justified integer); number may be between 1 and 200
		6-9 11-14 16-19,	The names of the reactants (up to three allowed); left-justified
		21-24, 26-29, 31-34, 36-39	The names of the products (up to four allowed); left-justified
		41-50	The rate constant at 298 K or the multiplicative factor for photolysis reactions (right-justified if E-format)
		51-60	The activation energy (in degrees K) if there is one (right-justified if E-format)
	7+(nonunity stoichiometric coefficient format)	1-4 7-10 13-16	The names of the reactants (up to 3 allowed); left-justified
		17-19	The identification number for the reaction (right-justified integer); MAX = 200
		20-24	Coefficient for 1st product (DF = 1.)
		25-28	Name of 1st product; left-justified
		29	An '*' in this column means that there will be additional (up to 6 more) products on the next card

TABLE 9 (continued)

Option	Card No.	Column	Contents
MECHANISM	4	31-35	Coefficient for 2nd product (DF = 1.)
		37-40	Name of 2nd product; left-justified
		43-47	Coefficient for 3rd product (DF = 1.)
		49-52	Name of 3rd product; left-justified
		55-64	The rate constant at 298 K or the photolysis multiplicative factor
		66-72	The activation energy (in degrees K)

The next card is used when more than 3 products are in the reaction.

		1-5	Coefficient for 4th product (DF = 1.)
		7-10	Name of 4th product; leus+gkpshuhib
		13-17	Coefficient for 5th product (DF = 1Z(
		19-22	Name of 5th product; left-justified
		25-29	Coefficient for 6th product (DF = 1.)
		31-34	Name of 6th product; left-justified
		37-41	Coefficient for 7th product (DF = 1.)
		43-46	Name of 7th product; left-justified
		49-53	Coefficient for 8th product (DF = 1.)
		55-58	Name of 8th product; left-justified
		61-65	Coefficient for 9th product (DF = 1.)
		67-70	Name of 9th product; left-justified

TABLE 9 (continued)

Option	Card No.	Column	Contents
ZENITH*			Revise or input photolysis rates as a function of solar zenith angle. This option is required when an optional mechanism is used. This option can also be used with the default mechanism (1) to vary the photolysis rates for species besides O_3, FORM, and ALD2 in a fashion independent from NO_2 photolysis or (2) to modify the default values for the zenith angle dependence of NO_2, O_3, FORM, and ALD2. Note that photolytic reactions that vary with zenith angle in a fashion similar to NO_2 need not be entered.
	1	1-4	ZENI
		5-10	Not read
		11-20	Number of photolysis reactions with zenith angle dependence.
			The next two cards are repeated for each photolysis reaction. The order of the photolysis rates represents values for the following zenith angles: 0., 10., 20., 30., 40., 50., 60., 70., 78., 86.
	2	1-10	Photolysis reaction number
		11-20 21-30 31-40 41-50 51-60 61-70	Photolytic ratios relative to NO_2 for the first six zenith angles.
	3	1-10 11-20 21-30 31-40	Photolytic ratios relative to NO_2 for the last four zenith angles.

---

* Default values for O_3, FORM, and ALD2 are shown in Table 4 (Section 4). The default values for NO_2 are shown in Table 3 (Section 4).

TABLE 9 (continued)

Option	Card No.	Column	Contents
TITLE	Input a new title. If this option is not activated, the default title is "Standard Ozone Isopleth Conditions."		
	1	1-4	TITL
	2	1-72	The title can be placed anywhere in card between columns (cc) 1-72

TABLE 9 (continued)

Option	Card No.	Column	Contents
PLACE	Input city-specific information on light intensity. Default values correspond to Los Angeles on 21 June 1975.		
	1	1-4	PLAC
		11-20	Latitude, in decimal degrees north of the equator (DF = 34.058)
		21-30	Longitude, in decimal degrees west of Greenwich meridian (DF = 118.250)
		31-40	The time zone, in hours from Greenwich mean time (DF = 8.0)
		41-50	The year (DF = 1975)
		51-60	The month of year (DF = 6)
		61-70	The numerical day of month (DF = 21)
	2 (optional)	1-24	The name of the place can be entered anywhere in cc 1-24. Include this card only if a new value is entered for the latitude or longitude on the previous card

TABLE 9 (continued)

Option	Card No.	Column	Contents
MIXING	Option for use when date on hourly mixing heights are available. Mixing heights are read for the initial height and the height at the end of each hour. If dilution occurs for n hours, there should be n+1 mixing heights.		
	1	1-4	MIXI
		11-20	Number of hours (n) of dilution (MAX = 24)
		21-30	Mixing height at time t = 0
		31-40	Mixing height at time t = 1 hr
		41-50	Mixing height at time t = 2 hr
		51-60	Mixing height at time t = 3 hr
		61-70	Mixing height at time t = 4 hr
		71-80	Not read
			If more than 4 hours of dilution, continue on next card
	2+ (optional)	1-10	Continuation of mixing heights
		.	
		.	
		.	
		61-70	
		71-80	Not read

TABLE 9 (continued)

Option	Card No.	Column	Contents
DILUTION	Read site-specific information on initial and final mixing heights. Dilution is calculated using the characteristic curve.		
	1	1-4	DILU
		11-20	Initial mixing height, Z1, in any units (DF = 510 m)
		21-30	Final mixing height, Z2, in same units as initial mixing height (DF = 630 m)
		31-40	Starting time of mixing height change (2400 hour) (DF = 800)
		41-50	Ending time of mixing height change (2400 hour) (DF = 1500)
		51-60	Dilution rate in percent per hour before and after the mixing height change (DF = 0)
		61-80	Not read

TABLE 9 (continued)

Option	Card No.	Column	Contents
TEMPERATURE	A varying temperature profile may be used during the simulation with this option. Temperature values should be in units of degrees K. Values are read for the initial time and at the end of each hour. If there are n hours, there should be n+1 temperature values.		
	1	1-4	TEMP (DF = 303 K)
		11-20	Number of hours (n) of varying temperature (MAX = 24)
		21-30	Temperature at time t = 0
		31-40	Temperature at time t = 1 hr
		41-50	Temperature at time t = 2 hr
		51-60	Temperature at time t = 3 hr
		61-70	Temperature at time t = 4 hr
		71-80	Not read
			If more than 4 hours of values, continue on next card
	2+ (optional)	1-10	Continuation of temperature values
		.	
		.	
		.	
		61-70	
		71-80	Not read

TABLE 9 (continued)

Option	Card No.	Column	Contents
TRANSPORT	Option for site-specific information on O_3, NO_2, NMOC transported in the surface layer and in the air aloft that is entrained as the inversion rises. (If TRAN option is not used, concentration of transported species is 0.)		
	1	1-4	TRAN
		11-20	Transport ozone concentration in the surface layer
		21-30	Ozone entrained from aloft
		31-40	If nonzero and positive:* Transported NMOC in the surface layer. If nonzero and negative: Number of NMOC species in the 0600-0900 mix
		41-50	If nonzero and positive:* Total NMOC entrained from aloft. If nonzero and negative: Number of NMOC species in the 0600-0900 mix
		51-60	Transported NO_2 in the surface layer
		61-70	NO_2 entrained from aloft
		71-80	Not read
	2 (optional)	1-10	If a nonzero negative value is entered in columns 31-40 of the TRAN card, the total NMOC transported in the surface layer is entered here (ppmC).
		11-20 . . . 61-70	The fraction of the total NMOC for each of the organic species transported in the surface layer (should be in the same order as listed in the MECH option) Continue on next card (if necessary)
		71-80	Not read

---

* Can only be used with the CBM-X. The default carbon fractions for NMOC transport in the surface layer and for NMOC aloft are given in Table 5, Section 4.

TABLE 9 (continued)

Option	Card No.	Column	Contents
TRANSPORT	3 (optional)	1-10	If a nonzero negative value is entered in columns 41-50 of the TRAN card, the total NMOC entrained from aloft is entered here (ppmC)
		11-20 . . . 61-70	The fraction of the total NMOC entrained for each of the organic species entrained from aloft. Continue on next card (if necessary)
		71-80	Not read

TABLE 9 (continued)

Option	Card No.	Column	Contents
INITIAL	Molecular concentrations of species other than O_3, NO_2, and NMOC that are transported in the surface layer can be entered with this card.		
	1	1-4	INIT
		11-20	Number of transported species with nonzero concentrations (DF = 0; MAX = 80)
		21-80	Not read
	2	1-4 11-14 21-24 31-34 41-44 51-54 61-64	The list names of the transported species with nonzero concentrations (continue on next card if necessary)
		65-80	Not read
	3	1-10 11-20 . . . 61-70	The molecular concentrations for the species listed on the previous card(s) (ppm)
		71-80	Not read

TABLE 9 (continued)

Option	Card No.	Column	Contents
ALOFT	Molecular concentrations of species other than NMOC, NO_x and O_3 in the aloft layer can be entered with this card.		
	1	1-4	ALOF
		11-20	Number of species with nonzero aloft concentrations (DF = 0; MAX = 10)
		21-80	Not read
	2	1-4 11-14 21-24 31-34 41-44 51-54 61-64	The list of names of the species with nonzero aloft concentrations
		65-80	Not read
	3	1-10 11-20 . . . 61-70	The aloft molecular concentrations for the species listed on the previous card (ppm)
		71-80	Not read

TABLE 9 (continued)

Option	Card No.	Column	Contents
BACKGROUND	Background concentrations of NMOC, NO_2 and O_3 can be set with this option. Surface layer and aloft conditions of NMOC, NO_2, and O_3 above background values are changed proportional to the reduction in initial NMOC or NO_x. (If background option is not used, the minimum background levels are zero.)		
	1	1-4	BACK
		11-20	Background concentration of O_3 (ppm)
		21-30	If nonzero and positive: The background concentration of NMOC (ppmC) for the CBM-X chemistry If nonzero and negative: The number of organic species in the optional mechanism; read next card
		31-40	Background concentration of NO_2 (ppm)
	2	1-10	Background concentration of NMOC (ppmc)
		11-20 21-30 31-40 41-50 51-60	The fraction of the total background NMOC for each of the organic species (should be in the same order as listed in the MECH option)
		61-70	Continue on next card (if necessary)

TABLE 9 (continued)

Option	Card No.	Column	Contents
EMISSIONS	Input city-specific information on post-0800 emissions.		
	1	1-4	EMIS
		11-20	The number of hours for which emission fractions are to be input, from 1.0 to 24.0 (DF = 0). This number should be coded as positive if the same fractions for NMOC and NO_x are to be used. It should be coded as negative if different fractions are to be used
		21-30	NMOC or NMOC and NO_x emission fraction for hour 1 (DF = 0). If all NMOC fractions are to be set to zero, enter any negative number and skip to record 2
		31-40	NMOC or NMOC and NO_x emission fraction for hour 2 (DF=0)
		. . .	
		61-70	NMOC or NMOC and NO_x emission fraction hour 5 (DF = 0)
	The following card(s) is included and repeated if more than five hours of emissions are specified.		
	2 (optional)	1-10	NMOC or NMOC and NO_x emission fraction for hour 6
		11-20	NMOC or NMOC and NO_x emission fraction for hour 7
		. . .	
		61-70	NMOC or NMOC and NO_x emission fraction for hour 12
	The next card(s) is included when separate NMOC and NO_x fractions are specified. The next card is repeated when the number of hours of emissions is greater than 7.		
	3 (optional)	1-10	NO_x emission fraction for hour 1. If all NO_x fractions are set to zero, then any negative number should be entered, and no further entries are required

TABLE 9 (continued)

Option	Card No.	Column	Contents
EMISSIONS		11-20	NO_x emission fraction for hour 2
		⋮	
		61-70	NO_x emission fraction for hour 7
	4 (optional)	1-10	NO_x emission fraction for hour 8
		11-20	NO_x emission fraction for hour 9
		⋮	
		61-70	NO_x emission fraction for hour 14

TABLE 9 (continued)

Option	Card No.	Column	Contents
MASSEMISS	Used to supply mass emission densities through which post-0800 emission fractions are computed		
	1	1-4	MASS
		11-20	Number of hours of emissions (max = 15.)
		21-30	Initial NMOC concentration used to compute NMOC emission fractions, ppmC
		31-40	Initial NO_x concentration used to compute NO_x emission fractions, ppm
		41-50	Mixing height at start of simulation, in meters
	The next card is repeated if more than 7 hours of emissions are specified. The number of entries must equal the number of hours specified on card 1.		
	2	1-10	VOC emission density for hour 1, kg/km^2
		11-20	VOC emission density for hour 2, kg/km^2
		.	
		.	
		.	
		61-70	VOC emission density for hour 7, kg/km^2
	The next card is repeated if more than 7 hours of emissions are specified. The number of entries must equal the number of hours specified on card 1.		
	3	1-10	NO_x emission density for hour 1, kg/km^2
		11-20	NO_x emission density for hour 2, kg/km^2
		.	
		.	
		.	
		61-70	NO_x emission density for hour 7, kg/km^2

TABLE 9 (continued)

Option	Card No.	Column	Contents
MOLEMISS	Incorporate site-specific information on emissions of up to 5 species including VOC and NO_x.		
	1	1-4	MOLE
		11-20	Number of hours during which emissions occur; from 1 to 24 (DF = 0)
		21-30	Number of species that have emission rates (MAX = 5)
		31-40	If nonzero: The initial mixing height used for conversion of moles to ppm units (units should be consistent with the initial mixing height value entered in the DILU or MIXI options)
		41-50	If nonzero, the horizontal area used to convert emissions in moles to ppm units (units for the area should be consistent with the mising height units)
	The next set of cards is repeated for each species with emissions.		
	2	1-4	Species name (use VOC for VOC emissions, NOX for nitrogen oxides emissions)
		11-20 21-30 . . .	Emission rates in units of ppm/hr or moles/hr (ppmC or moles C for VOC emissions)
		61-70	If more than 5 hours of continuous emissions are to be entered, continue on next card.

TABLE 9 (continued)

Option	Card No.	Column	Contents
DEPOSITION	Incorporate information on species deposition.		
	1	1-4	DEPO
		11-20	Number of hours during which deposition occurs; from 1 to 24; DF = 0
		21-30	Number of species that have deposition rates; MAX = 5
	The next set of cards is repeated for each species with deposition rates.		
	2	1-4	Species name (use NMOC for NMOC deposition) (NO and NO_2 deposition are treated separately)
		11-20 21-30 . . . 61-70	Deposition velocity in units of cm/s
	If more than 5 hours of deposition are to be entered, continue on next card.		

TABLE 9 (continued)

Option	Card No.	Column	Contents
REACTIVITY*	Contains site-specific information on organic reactivity and NO_2/NO_x ratio for the initial 6-9 AM mix and the VOC and NO_x emissions.		
	1	1-4	REAC
		5-10	Not read
		11-20	The number of primary organic species in the mechanism
		21-30	The NO_2/NO_x fraction
	2	1-10 . . . 61-70	The reactivity for each of the organic species (up to 7 on a card) represented as the fractions of total NMOC. Continue on next card (if necessary)
		71-80	Not read

---

* If the REACTIVITY option is not used, the default fractions are those shown in Table 7, Section 4.

TABLE 9 (continued)

Option	Card No.	Column	Contents
TIME	Reset starting and ending times for simulations with this card.		
	1	1-4	TIME
		5-10	Not read
		11-20	Starting time for simulations based on 24-hour clock (DF = 800)
		21-30	Ending time for simulations (DF = 1800). Note: Maximum difference is 24 hours
		31-80	Not read

TABLE 9 (continued)

Option	Card No.	Column	Contents
RATE	Rate constant changes are implemented with this card.		
	1	1-4	RATE
		5-10	Not read
		11-20	Number of rate constants to be changed
		21-30	Special option for testing emissions, photolysis, dilution, etc. A nonzero number sets all reaction rate constants to zero except photolysis reactions
	2 (optional)	1-10 . . . 61-70	Reactions with rate constants to be changed (each reaction number in each 10-column field)
		71-80	Not read
	3 (optional)	1-10 . . . 61-70	List of the new rate constants (must be in the same order as the reactions from previous card). Each rate constant in each 10-column field (right-justified if E format)
		71-80	Not read

TABLE 9 (continued)

Option	Card No.	Column	Contents
SPECIES	This card allows the user to plot isopleths for any species found in the kinetic mechanism or to plot concentration-time profiles for species besides O_3 if the CALCULATE option is used.		
	1	1-4	SPEC
		11-20	Number of species to be plotted (DF = 1)
		21-80	Not read
		1-4 11-14 21-24 31/34 41-44	The alphanumeric symbol of the species of interest; left-justified (DF = 03 [ozone])
		45-80	Not read

TABLE 9 (continued)

Option	Card No.	Column	Contents
ACCURACY	Increase or reduce the mathematical accuracy of the isopleth diagram by using more or fewer simulations, more or less accurate interpolation, etc.		
	1	1-4	ACCU
		11-20	Number of constant initial NMOC/NO$_x$ ratios (radial lines form the origin of the isopleth diagram) on which simulations are to be performed, any odd number from 1. to 19.; (DF = 11)
		21-30	Number of simulations per radial line, from 1. to 8.; (DF = 5)
		31-40	Error tolerance in the numerical integration routine, from 0.1 to 0.00001; (DF = 0.01)
		41-50	Tension factor for hyperbolic spline functions used in first stage of interpolation from 0.001 to 50.; (DF = 1)
		51-60	Tension factor for hyperbolic spline functions used in plotting isopleth lines (high tensions lead to straight lines drawn between the points obtained from the first stage), from 0.001 to 50.; (DF = 1)
		61-70	If any nonzero value is entered in this field, simulations will terminate after any ozone maximum; no entry produces results over the total simulation period

TABLE 9 (continued)

Option	Card No.	Column	Contents
ALREADY	Include results from a previous run.		
	1	1-4	ALRE
		11-20	Number of previous simulations to be input If the number is positive, then read the following cards. If the number is negative, then read previous simulation results from an external file
	2	1-10	NMOC concentration
		11-20	NO_x concentration
		21-30	Maximum one-hour average ozone concentration, ppm
		31-40 41-50 51-60 61-70	Maximum one-hour average species concentrations, ppm. These values are optional depending on the number of species declared on the SPECIES card.

TABLE 9 (continued)

Option	Card No.	Column	Contents
PLOT	Activates the drawing of the isopleth diagram on an off-line plotter.		
	1	1-4	PLOT
		11-20	Scaling factor for the location of labels for each ozone isopleth. The value should be between 0.1 and 0.8.; (DF = 0.6)
		21-30	If nonzero, a grid is overlaid onto the diagram. If the value is positive and nonzero, a grid is overlaid on the diagram using a different color pen (if available) If the value is negative, a grid with line of different patterns (e.g., dot-dash) is overlaid on the plot. The absolute value of this number corresponds to different patterns and textures
		31-40	Length (in inches) of the abscissa (NMOC scale) of the isopleth diagram; (DF = 8.5)
		41-50	Length (in inches) of the ordinate (NO_x scale) of the isopleth diagram; (DF = 5.95)
		51-60	Size (in inches) of the numbers to be printed on the axes and of the characters in the title; (DF = 0.10)
		61-70	The size (in inches) of the labels on the ozone isopleths and the division marks on the axis; (DF = 0.07)

TABLE 9 (continued)

Option	Card No.	Column	Contents
CALCULATE	Perform a single simulation with the initial NMOC and NO_x concentrations specified on this card.		
	1	1-4	CALC
		11-20	NMOC concentration
		21-30	NO_x concentration
		31-40	Information option; entry of any positive value will result in printing of the computed concentrations of all species, the rate of change of all species, reaction rates, etc. Photolysis constants are also printed
		41-50	Time (in minutes) from the beginning of the simulation at which computed concentrations of all species in the kinetic mechanism are to be printed; (DF = 60)
		51-60	Time step (in minutes) for subsequent printing of concentrations; (DF = 60)

TABLE 9 (continued)

Option	Card No.	Column	Contents
EKMA	Used to perform a VOC emission requirement calculation		
	1	1-4	EKMA
		11-20	Base-case ozone concentration, ppm
		21-30	NMOC/NO_x ratio
		31-40	Percentage change in NO_x emissions; positive number for increase, negative number for decrease (DF = 0)
		41-50	Change in transport option indicator; if nonzero, input record 2 is required (DF = 0)
		51-60	Option to generate report of change in ozone as a function of change in VOC emissions; if 1., generate tabular report; if 2., generate tabular report and write results to file. (DF = 0., i.e., no report or file generated)
		61-70	Flag to do a calculation at a specified NMOC level. A negative value means that only this calculation will be done. A positive value means that the attainment calculation will be performed in addition to the calculation at the specified NMOC level.
	The next card is included only if a nonzero entry is specified for the transport option (41-50) and/or the flag option (61-70)		
	2 (optional)	1-10	Concentration of ozone transported in surface layer for post-control conditions, ppm; (DF = base-case level) A negative value activates the use of the future ozone transport estimate curves shown in Figure 4. (A value less than -100 activates the use of the dotted line shown in Figure 4.)
		11-20	Concentration of ozone transported aloft for post-control conditions, ppm; (DF = base-case level) A negative value activates the use of the future ozone transport estimate curves shown in Figure 4. (A value less than -100 activates the use of the dotted line shown in Figure 4.)

TABLE 9 (continued)

Option	Card No.	Column	Contents
EKMA	2	21-30	Concentration of NMOC transported in the surface layer for post-control conditions, ppmC; (DF = base-case level) A negative value represents the median contribution factor as described in Appendix B of EPA (1981).
		31-40	Concentration of NMOC transported aloft for post-control conditions, ppmC; (DF = base-case level) A negative value represents a 40% reduction in present-day NMOC aloft
		41-50	Concentration of NO_x transported in surface layer for post-control conditions, ppm; (DF = base-case level)
		51-60	Concentration of NO_x transported aloft for post-control conditions, ppm; (DF = base-case level)
		61-70	Change in NMOC level (percent) for specific calculation after the base-year ozone is estimated. (Used only if column 61-70 of Card 1 is non-zero.)

TABLE 9 (continued)

Option	Card No.	Column	Contents
ISOPLETH	Construct an ozone isopleth diagram according to the input parameters. Default isopleths are 0.08, 0.12, 0.16, 0.20, 0.24, 0.28, 0.30, 0.32, 0.34, 0.36 and 0.40 ppm.		
	1	1-4	ISOP
		11-20	Maximum NMOC concentration on abscissa of isopleth diagram; (DF = 2.0 ppmC)
		21-30	Maximum NO_x concentration on ordinate of isopleth diagram; (DF = 0.28 ppm)
		31-40	Number of ozone isopleths to be drawn, from 1. to 20.; (DF = 11)
		41-50	Any nonzero value will activate the printing of solar noon and the time of the center of the maximum one-hour average ozone concentration for each simulation
	2 (optional)	1-10	Ozone concentration of 1st isopleth, ppm
		11-20	Ozone concentration of 2nd isopleth, ppm
		21-30	Ozone concentration of 3rd isopleth, ppm
		31-40	Ozone concentration of 4th isopleth, ppm
		41-50	Ozone concentration of 5th isopleth, ppm
		51-60	Ozone concentration of 6th isopleth, ppm
		61-70	Ozone concentration of 7th isopleth, ppm

TABLE 9 (concluded)

Option	Card No.	Column	Contents
ISOPLETH	3 (optional)	1-10	Ozone concentration of 8th isopleth, ppm
		. . .	
		61-70	Ozone concentration of 14th isopleth, ppm
	4 (optional)	1-10	Ozone concentration of 15th isopleth, ppm
		. . .	
		51-60	Ozone concentration of 20th isopleth, ppm

TABLE 9 (continued)

Option	Card No.	Column	Contents
bbbb	A blank card must follow all input cards to terminate the program.		
	1	1-4	Blanks

TABLE 10. FILES USED BY OZIPM-3.

File	FORTRAN Unit*	Read(R)/ Write(W)	Comment
Input file	5	R	The card input deck
Output file	6	W	The output of the OZIPM-3 results
ALREADY file	9	W	The results of each simulation on a diagram point are written to this file for later use
ALREADY file	8	R	File of results from a previous run used to continue an isopleth simulation or redo the isopleth
PLOT file (optional)	--	W	The file to which CALCOMP or offline plots are written. The file unit is dependent on the computer system

---

* Each of the unit numbers can be changed in the OZIPM-3 program by modifying the following statement in the BLOCK DATA routine:

```
DATA IN/S/, OUT/6/, IALN/9/, IALL/8/.
```

6 EXAMPLES OF OZIPM RUNS

Five examples of how to use OZIPM-3 with the CBM-X and optional mechanisms are presented in this section. Exhibits 1 through 10* show the input and output files for each example. The examples are discussed in detail below.

Example 1

Example 1 illustrates the use of the default CBM-X mechanism with a set of city-specific information described by PLACE, DILUTION, EMISSIONS, and TRANSPORT options. Exhibit 1 shows the input file for this example. (The first four lines of code in this exhibit were used to orient the user by providing column numbers. The actual input stream begins on line 5.) A single simulation is performed using the CALCULATE option at a NMOC value of 1.1 ppmC and a NO_x value of 0.12 ppm. Also note that there is a nonzero value in columns 31-40 of the CALC card, which will result in a detailed printout of the simulation. The SPECIES option is used in this simulation so that plots of maximum hourly-averaged concentrations of NO_2 and PAR can be obtained along with the plot of the maximum hourly-averaged O_3 concentration.

The output from this simulation is shown in Exhibit 2. The first page of the output describes the versions of OZIPM-3 being used. The second page is a printout of the input stream. This feature is provided so that users may readily review the input information associated with the simulation output. The default mechanism and the photolysis rates are printed next because a value of -1 was placed on the MECHANISM option. The next two pages are header pages that describe the inputs used in this simulation. The following pages contain the detailed simulation results for each hour of the simulation. At the end of the simulation is a summary of the maximum O_3, NO_2, and PAR concentrations found in the simulation. Three plots (one each for O_3, NO_2, and PAR) in the output show the temporal behavior for each species of interest.

---

* For the convenience of the user, Exhibits 1 through 10 are presented at the end of this section.

Example 2

Example 2 illustrates the use of the CALCULATE option for a chemical mechanism other than the default CBM-X mechanism. Exhibit 3 shows the input deck for this simulation. The example shown here uses the CBM-3 mechanism described by EPA (1984); this example is comparable to the example shown in that document. The chemical mechanism is implemented through the use of the MECHANISM card. Since the chemical reactions are input in the CHEMK format, a flag (or nonzero) value is entered in columns 41-50 of the MECHANISM card. Following the MECHANISM card is (1) the list of photolysis reactions, (2) the list of the organic species, and (3) the carbon number of each organic species. The chemical reactions are input next. Note that the photolysis reactions listed (line 7 of Exhibit 3) do not have to be in consecutive order.

The ZENITH option follows the MECHANISM option. Note that the ZENITH option contains a set of values to adjust the NO_2 photolysis (reaction 1) back to the NO_2 photolysis used in previous versions of OZIPP and OZIPM. The zenith angle dependence for each photolysis reaction is entered beginning at 0(zero) degrees. Note that only six photolysis reactions are input even though there are a total of seven photolysis reactions. Reaction 67 has a zenith angle dependence similar to that of NO_2 photolysis. Since the Reaction 67 photolysis rate constant is a constant ratio to NO_2 photolysis, its zenith angle dependence does not need to be input with the ZENITH option.

Following the ZENITH option are the city-specific options described in Example 1. The only difference is in the TRANSPORT option, which requires defining the organic fractions as shown in Table 10, Section 5. The output is shown in Exhibit 4. The output formats are similar to those given in Example 1 except that the chemical mechanism is printed.

Example 3

Example 3 illustrates the use of the EKMA option to predict the actual reduction in VOC emissions needed to reach the NAAQS of 0.12 ppm. Exhibit 5 shows the input file for this example. The design ozone is 0.171 ppm, the $NMOC/NO_x$ ratio is 9.5, and the NO_x emissions are reduced by 10.7 percent for the future year. The nonzero flag in columns 41-50 of the EKMA option represents a change in transport concentrations in the future year. The nonzero value in columns 61-70 tells OZIPM-3 to do a calculation for the future year at a specific NMOC level. The next card after the EKMA card determines the change in transport for the future year. The first two fields, columns 1-10 and 11-20, specify the future-year ozone transported in the surface layer and aloft. A negative value is entered to tell OZIPM-3 to use the standard ozone curves described in EPA (1981) and shown in Figure 4.

The future-year NMOC transported in the surface layer and aloft are input in columns 21-30 and 31-40, followed by the future NO_x transported in the surface layer and aloft (columns 41-50 and 51-60). The last field (columns 61-70) contains the specific NMOC level at which the future calculation will be performed. The output for this example is shown in Exhibit 6. The output formats are similar to the output from the previous examples except that the simulations required to make the VOC requirement estimate are printed. Note that OZIPM-3 will search for the NMOC and NO_x level along the NMOC/NO_x ratio until it finds the design ozone of 0.171 ppm. Then it performs the future year estimate to obtain the VOC control requirement.

Example 4

Example 4 is similar to Example 3 except that the NMOC transported in the surface layer must be reduced due to upwind contributions. The procedure outlined in this example is that described in Appendix B of the 1981 EPA guidelines. Exhibit 7 shows the input file for this example. The card following the EKMA card contains the upwind NMOC median contribution factor of 0.32. The contribution factor is entered as a negative number to distinguish it from an absolute concentration. The output for this example is shown in Exhibit 8.

Example 5

Example 5 demonstrates many of the OZIPM-3 options in one computer run. Exhibit 9 shows the input file for this example. The chemical mechanism used in this example is a condensed form of the default CBM-X mechanism (see Whitten, Johnson, and Killus, 1985, for a detailed discussion of this mechanism). The condensation of the CBM-X mechanism was achieved by combining many of the reactions presented in Appendix A using the stoichiometric coefficient format in OZIPM-3; the use of this format to condense a chemical mechanism allows the user to save computation time. In this example, the default CBM-X mechanism is reduced to 111 reactions (from 148). Note in Exhibit 9 the use of the more than three products per reaction format (e.g., lines 87 and 88). An ozone isopleth is also generated in this example. The output for this example is shown in Exhibit 10. The output contains the results of the single simulation performed for the CALCULATE option followed by the simulations performed for the ISOPLETH option. The ozone isopleth diagram is shown at the end of the output file. Note that the SPECIES option asked for three species (O_3, NO_2, and PAR). Thus, the simulations under the ISOPLETH option provide the maximum one-hour values for all three species. Since an isopleth can only be generated for the first species of interest, the user can generate an isopleth diagram for NO_2 or PAR through the use of the ALREADY option. The NO_2 or PAR values would be input instead of ozone.

EXAMPLE 1

CALC USING CBM-X

```
(     1)
(     2)          1         2         3         4         5         6         7
(     3) 123456789012345678901234567890123456789012345678901234567890123456789012
(     4)
(     5) MECH      -1.
(     6) TITL
(     7) EXAMPLE 1 - TEST RUN USING EKMA/CBM-X
(     8) PLACE     39.933    75.10     5.0       1980.     6.0       24.0
(     9) TEST CITY
(    10) DILU      250.      1235.               1600.
(    11) EMIS      -8.0      .17       .17       .17       .10       .02
(    12) .02       .02       .02
(    13) .35       .35       .35       .19       .03       .03       .03
(    14) .07
(    15) TRANS     .010      .070      .038      .04       0.0       0.0
(    16) SPEC      3.
(    17) O3        NO2       PAR
(    18) CALC      1.1       .12       1.
(    19)
(    20)     BLANK
```

Exhibit 1

```
****************************************
*                                      *
*   OZONE ISOPLETH PLOTTING PACKAGE    *
*     WITH OPTIONAL MECHANISMS         *
*                                      *
*            O Z I P M                 *
*                                      *
*           VERSION 3.1                *
*                                      *
*         SEPTEMBER, 1985              *
*                                      *
****************************************
```

Exhibit 2

```
THE INPUTS FOR THIS RUN ARE

         MECH       -1.
         TITL
         EXAMPLE 1 - TEST RUN USING EKMA/CBM-X
         PLACE      39.933     75.10      5.0        1980.      6.0        24.0
         TEST CITY
         DILU       250.       1235.                 1600.
         EMIS       -8.0       .17        .17        .17        .10        .02
         .02        .02        .02
         .35        .35        .35        .19        .03        .03        .03
         .07
         TRANS      .010       .070       .038       .04        0.0        0.0
         SPEC       3.
         O3         NO2        PAR
         CALC       1.1        .12        1.
```

```
THE REACTIONS                                                                    RATE CONSTANT  ACT. ENERGY(K)
  1        NO2                      =      NO   +    O                             1.000E 00      0.000E-01
  2        O                        =      O3                                      4.440E 06     -6.900E 02
  3        O3    +     NO           =      NO2                                     2.660E 01      1.430E 03
  4        O     +     NO2          =      NO                                      1.380E 04      0.000E-01
  5        O     +     NO2          =      NO3                                     2.320E 03     -6.000E 02
  6        O     +     NO           =      NO2                                     3.120E 03     -4.110E 02
  7        NO2   +     O3           =      NO3                                     4.740E-02      2.450E 03
  8        O3                       =      O1D                                     1.160E 00      0.000E-01
  9        O3                       =      O                                       4.200E-02      0.000E-01
 10        O1D                      =      O                                       4.290E 10     -1.000E 02
 11        O1D                      =      OH   +    OH                            6.520E 09      0.000E-01
 12        O3    +     OH           =      HO2                                     1.000E 02      9.400E 02
 13        O3    +     HO2          =      OH                                      3.000E 00      5.800E 02
 14        NO3   +     NO           =      NO2  +    NO2                           2.810E 04     -2.500E 02
 15        NO3   +     NO2          =      NO   +    NO2                           5.900E-01      1.230E 03
 16        NO3   +     NO2          =      N2O5                                    1.780E 03      6.000E 01
 17        N2O5                     =      HNO3 +    HNO3                          3.800E-02      0.000E-01
 18        N2O5                     =      NO3  +    NO2                           3.120E 00      1.084E 04
 19        NO    +     NO2          =      HNO2 +    HNO2                          3.200E-07      0.000E-01
 20        HNO2  +     HNO2         =      NO   +    NO2                           1.500E-05      0.000E-01
 21        HNO2                     =      NO   +    OH                            1.800E-01      0.000E-01
 22        NO2   +     OH           =      HNO3                                    1.630E 04     -5.600E 02
 23        NO    +     OH           =      HNO2                                    9.770E 03     -4.270E 02
 24        HO2   +     NO           =      OH   +    NO2                           1.230E 04     -2.400E 02
 25        NO    +     NO           =      NO2  +    NO2                           1.456E-04     -5.300E 02
```

```
THE REACTIONS                                                                    RATE CONSTANT  ACT. ENERGY(K)
 26      H202                   =     OH    +    OH                                1.400E-03      0.000E-01
 27      OH    +    H202        =     HO2                                          2.520E 03      1.870E 02
 28      OH    +    HNO2        =     NO2                                          9.770E 03      0.000E-01
 29      OH    +    HNO3        =     NO3                                          1.920E 02     -7.780E 02
 30      NO3                    =     NO2   +    O                                 2.600E 01      0.000E-01
 31      NO3                    =     NO                                           4.600E 00      0.000E-01
 32      HO2   +    HO2         =     H202                                         4.144E 03     -1.150E 03
 33      HO2   +    HO2         =     H202                                         4.360E 03     -5.800E 03
 34      HO2   +    NO2         =     PNA                                          1.630E 03     -6.170E 02
 35      PNA                    =     HO2   +    NO2                               5.120E 00      1.042E 04
 36      OH    +    CO          =     HO2                                          4.000E 02      0.000E-01
 37      FORM  +    HO2         =     FROX                                         1.480E 01      0.000E-01
 38      FORM  +    OH          =     HO2   +    CO                                1.500E 04      0.000E-01
 39      FORM                   =     HO2   +    HO2   +    CO                     1.100E 00      0.000E-01
 40      FORM                   =     CO                                           1.060E 00      0.000E-01
 41      FORM  +    O           =     OH    +    HO2   +    CO                     2.370E 02      1.550E 03
 42      FORM  +    NO3         =     HNO3  +    HO2   +    CO                     9.300E-01      0.000E-01
 43      FROX  +    NO          =     FACD  +    NO2   +    HO2                    1.040E 04      0.000E-01
 44      FROX                   =     HO2   +    FORM                              9.000E 01      0.000E-01
 45      ALD2  +    O           =     C2O3  +    OH                                6.360E 02      9.860E 02
 46      ALD2  +    OH          =     C2O3                                         2.400E 04     -2.500E 02
 47      ALD2  +    NO3         =     C2O3  +    HNO3                              3.700E 00      0.000E-01
 48      ALD2                   =     MEO2  +    HO2   +    CO                     1.110E 00      0.000E-01
 49      ALD2  +    HO2         =     MEO2  +    FORM                              5.000E 00      0.000E-01
 50      C2O3  +    NO          =     MEO2  +    NO2                               1.650E 04     -2.500E 02
```

```
THE REACTIONS                                                                     RATE CONSTANT  ACT. ENERGY(K)
 51     C203  +   NO2          =    PAN                                             9.000E 03     -2.500E 02
 52     PAN                    =    C203  +   NO2                                   2.220E-02      1.400E 04
 53     MEO2  +   NO2          =    MPNA                                            6.000E 03     -7.350E 02
 54     MPNA                   =    MEO2  +   NO2                                   9.200E 01      1.040E 04
 55     MEO2  +   NO           =    MEO   +   NO2                                   1.100E 04     -1.800E 02
 56     MEO   +   NO           =    MNIT                                            4.440E 04     -2.000E 02
 57     MEO   +   NO           =    FORM  +   HO2   +   NO                          1.920E 03      0.000E-01
 58     MEO   +   NO2          =    MEN3                                            2.220E 04      0.000E-01
 59     MEO                    =    FORM  +   HO2                                   3.760E 05      1.313E 03
 60     MEN3  +   OH           =    FORM  +   NO2                                   2.220E 03      3.600E 02
 61     MNIT  +   OH           =    FORM  +   NO                                    2.370E 03      3.400E 02
 62     MNIT                   =    MEO   +   NO                                    3.000E-01      0.000E-01
 63     MEO2  +   MEO2         =    MEO   +   MEO                                   1.750E 02     -2.200E 02
 64     MEO2  +   MEO2         =    FORM  +   MEOH                                  3.280E 02     -2.200E 02
 65     MEO2  +   C203         =    MEO   +   MEO2                                  4.400E 03      0.000E-01
 66     C203  +   C203         =    MEO2  +   MEO2                                  3.700E 03      0.000E-01
 67     MEO2  +   HO2          =    PROX                                            8.900E 03     -1.300E 03
 68     C203  +   HO2          =    PROX                                            9.600E 03      0.000E-01
 69     AONE                   =    MEO2  +   C203                                  4.000E-05      0.000E-01
 70     AONE  +   OH           =    ANO2                                            5.800E 02      0.000E-01
 71     ANO2  +   NO           =    NO2   +   FORM  +   C203                        1.200E 04      0.000E-01
 72     GLY                    =    CO    +   CO                                    5.200E-03      0.000E-01
 73     GLY                    =    CO    +   FORM                                  1.600E-03      0.000E-01
 74     GLY                    =    HO2   +   HO2   +   CO    +   CO                7.000E-04      0.000E-01
 75     GLY   +   OH           =    HO2   +   CO    +   CO                          1.500E 04      0.000E-01
```

```
THE REACTIONS
                                                                                    RATE CONSTANT  ACT. ENERGY(K)
 76     MGLY                 =   C2O3  +   HO2  +   CO                               2.000E-02     0.000E-01
 77     MGLY  +    OH        =   MGPX                                               2.600E 04     0.000E-01
 78     MGPX  +    NO        =   C2O3  +   NO2                                      1.200E 04     0.000E-01
 79     OH                   =   MEO2                                               2.100E 01     0.000E-01
 80     PAR   +    OH        =   RO2                                                1.500E 02     0.000E-01
 81     PAR   +    OH        =   RO2R                                               1.000E 03     0.000E-01
 82     RO2   +    NO        =   NO2   +   HO2  +   ALD2  +   X                     1.200E 04     0.000E-01
 83     RO2R  +    NO        =   NO2   +   ROR                                      1.200E 04     0.000E-01
 84     RO2R  +    NO        =   NTR                                                1.000E 03     0.000E-01
 85     ROR   +    NO2       =   NTR                                                2.200E 04     0.000E-01
 86     ROR                  =   KET   +   HO2                                      1.500E 05     0.000E-01
 87     ROR                  =   ALD2  +   D    +   X                               9.000E 04     7.000E 03
 88     ROR                  =   AONE  +   D    +   X     +   X                     2.400E 05     0.000E-01
 89     X     +    PAR       =                                                      1.000E 04     0.000E-01
 90     D     +    PAR       =   RO2                                                3.000E 03     0.000E-01
 91     D     +    PAR       =   AO2   +   X    +   X                               7.000E 03     0.000E-01
 92     D     +    KET       =   C2O3  +   X                                        1.000E 04     0.000E-01
 93     AO2   +    NO        =   NO2   +   HO2  +   AONE                            1.200E 04     0.000E-01
 94     KET                  =   C2O3  +   RO2  +   X     +   X                     3.000E-04     0.000E-01
 95     O     +    OLE       =   MEO2  +   C2O3 +   X                               3.000E 02     3.240E 02
 96     O     +    OLE       =   RO2   +   HO2  +   CO    +   X                     8.800E 02     3.240E 02
 97     O     +    OLE       =   ALD2                                               4.740E 03     3.240E 02
 98     OH    +    OLE       =   MEO2  +   ALD2 +   X                               4.200E 04    -5.370E 02
 99     O3    +    OLE       =   ALD2  +   CRIG +   X                               5.400E-03     0.000E-01
100     O3    +    OLE       =   FORM  +   MCRG +   X                               5.400E-03     1.897E 03
```

```
THE REACTIONS                                                                          RATE CONSTANT  ACT. ENERGY(K)
101      O3    +    OLE          =      ALD2  +    HOTA  +    X                         3.600E-03      1.897E 03
102      O3    +    OLE          =      FORM  +    HTMA  +    X                         3.600E-03      1.897E 03
103      NO3   +    OLE          =      PNO2                                            1.140E 01      0.000E-01
104      O     +    ETH          =      MEO2  +    HO2   +    CO                        1.080E 03      8.000E 02
105      OH    +    ETH          =      MEO2  +    FORM                                 1.200E 04     -3.820E 02
106      O3    +    ETH          =      FORM  +    CRIG                                 1.000E-03      2.840E 03
107      O3    +    ETH          =      FORM  +    HOTA                                 1.700E-03      2.840E 03
108      HOTA                    =                                                      2.500E 01      0.000E-01
109      HOTA                    =      CO                                              5.800E 01      0.000E-01
110      HOTA                    =      HO2   +    HO2                                  1.000E 01      0.000E-01
111      HOTA                    =      FACD                                            7.000E 00      0.000E-01
112      HTMA                    =                                                      2.000E 02      0.000E-01
113      HTMA                    =      MEO2  +    CO    +    OH                        4.000E 02      0.000E-01
114      HTMA                    =      MEO2  +    HO2                                  3.200E 02      0.000E-01
115      HTMA                    =      HO2   +    CO    +    FORM  +    HO2            8.000E 01      0.000E-01
116      CRIG  +    NO           =      FORM  +    NO2                                  1.000E 04      0.000E-01
117      CRIG  +    NO2          =      FORM  +    NO3                                  1.000E 03      0.000E-01
118      CRIG                    =      FACD                                            1.200E 02      0.000E-01
119      CRIG  +    FORM         =      OZD                                             3.000E 01      0.000E-01
120      CRIG  +    ALD2         =      OZD                                             3.000E 01      0.000E-01
121      MCRG  +    NO           =      ALD2  +    NO2                                  1.000E 04      0.000E-01
122      MCRG  +    NO2          =      ALD2  +    NO3                                  1.000E 03      0.000E-01
123      MCRG                    =      ACAC                                            1.200E 02      0.000E-01
124      MCRG  +    FORM         =      OZD                                             3.000E 01      0.000E-01
125      MCRG  +    ALD2         =      OZD                                             3.000E 01      0.000E-01
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```
THE REACTIONS                                                                       RATE CONSTANT  ACT. ENERGY(K)
126       PNO2  +    NO              =    DNIT                                        1.000E 03     0.000E-01
127       PNO2  +    NO              =    NTR   +   HO2   +   NO2                     1.000E 04     0.000E-01
128       TOL   +    OH              =    OPEN  +   GLY                               5.500E 03     0.000E-01
129       TOL   +    OH              =    PHEN  +   HO2   +   PAR                     3.500E 03     0.000E-01
130       TOL   +    OH              =    BO2                                         7.500E 02     0.000E-01
131       OPEN  +    NO              =    NO2   +   HO2   +   MGLY  +   GLY           1.000E 04     0.000E-01
132       PHEN  +    NO3             =    PHO   +   HNO3                              1.400E 04     0.000E-01
133       BZA   +    OH              =    BZO2                                        2.000E 04     0.000E-01
134       BZO2  +    NO2             =    PBZN                                        2.500E 03     0.000E-01
135       BZO2  +    NO              =    NO2   +   PHO2  +   CO                      3.700E 03     0.000E-01
136       BO2   +    NO              =    NO2   +   BZA   +   HO2                     1.200E 04     0.000E-01
137       PBZN                       =    BZO2  +   NO2                               2.200E-02     1.400E 04
138       BZA                        =    PROD                                        4.000E-03     0.000E-01
139       PHO   +    NO2             =    NPHN                                        2.000E 04     0.000E-01
140       PHO2  +    NO              =    NO2   +   PHO                               1.200E 04     0.000E-01
141       XYL   +    OH              =    XYLO                                        2.000E 03     0.000E-01
142       XYLO  +    NO              =    NO2   +   HO2   +   TLA                     1.200E 04     0.000E-01
143       TLA   +    OH              =    TLO2                                        2.000E 04     0.000E-01
144       TLO2  +    NO              =    NO2   +   PHO   +   PAR   +   PAR           4.000E 03     0.000E-01
145       XYL   +    OH              =    HO2   +   PHEN  +   PAR   +   PAR           1.000E 04     0.000E-01
146       XYL   +    OH              =    OPEN  +   MGLY                              2.400E 04     0.000E-01
147       OH                         =    HO2                                         8.800E 01     0.000E-01
148       NR                         =    NR                                          1.000E 00     0.000E-01
```

THE FOLLOWING PHOTOLYSIS RATE CONSTANTS ARE USED

REACTION NO.	SPECIES	ZENITH ANGLE (DEG) 0	10	20	30	40	50	60	70	78	86
1	NO2	6. 00E-01	5. 95E-01	5. 86E-01	5. 64E-01	5. 32E-01	4. 85E-01	4. 09E-01	2. 88E-01	1. 55E-01	3. 49E-02
8	O3	3. 24E-03	3. 14E-03	2. 83E-03	2. 31E-03	1. 71E-03	1. 08E-03	5. 26E-04	1. 59E-04	3. 78E-05	4. 53E-06
9	O3	2. 52E-02	2. 50E-02	2. 46E-02	2. 37E-02	2. 23E-02	2. 04E-02	1. 72E-02	1. 21E-02	6. 52E-03	1. 47E-03
21	HNO2	1. 08E-01	1. 07E-01	1. 05E-01	1. 02E-01	9. 57E-02	8. 73E-02	7. 36E-02	5. 19E-02	2. 79E-02	6. 28E-03
26	H2O2	8. 40E-04	8. 33E-04	8. 20E-04	7. 90E-04	7. 44E-04	6. 79E-04	5. 72E-04	4. 03E-04	2. 17E-04	4. 89E-05
30	NO3	1. 56E 01	1. 55E 01	1. 52E 01	1. 47E 01	1. 38E 01	1. 26E 01	1. 06E 01	7. 49E 00	4. 03E 00	9. 07E-01
31	NO3	2. 76E 00	2. 74E 00	2. 69E 00	2. 60E 00	2. 45E 00	2. 23E 00	1. 88E 00	1. 33E 00	7. 14E-01	1. 61E-01
39	FORM	1. 79E-03	1. 77E-03	1. 68E-03	1. 54E-03	1. 33E-03	1. 07E-03	7. 37E-04	3. 96E-04	1. 56E-04	2. 65E-05
40	FORM	2. 39E-03	2. 37E-03	2. 30E-03	2. 15E-03	1. 95E-03	1. 68E-03	1. 30E-03	7. 91E-04	3. 77E-04	8. 06E-05
48	ALD2	4. 29E-04	4. 12E-04	3. 93E-04	3. 38E-04	2. 79E-04	2. 01E-04	1. 24E-04	6. 11E-05	1. 86E-05	2. 09E-06
62	MNIT	1. 80E-01	1. 79E-01	1. 76E-01	1. 69E-01	1. 60E-01	1. 46E-01	1. 23E-01	8. 65E-02	4. 66E-02	1. 05E-02
69	ACNE	2. 40E-05	2. 38E-05	2. 34E-05	2. 26E-05	2. 13E-05	1. 94E-05	1. 63E-05	1. 15E-05	6. 21E-06	1. 40E-06
72	GLY	3. 12E-03	3. 09E-03	3. 05E-03	2. 93E-03	2. 77E-03	2. 52E-03	2. 13E-03	1. 50E-03	8. 07E-04	1. 81E-04
73	GLY	9. 60E-04	9. 52E-04	9. 37E-04	9. 03E-04	8. 51E-04	7. 76E-04	6. 54E-04	4. 61E-04	2. 48E-04	5. 58E-05
74	GLY	4. 20E-04	4. 17E-04	4. 10E-04	3. 95E-04	3. 72E-04	3. 40E-04	2. 86E-04	2. 02E-04	1. 09E-04	2. 44E-05
76	MGLY	1. 20E-02	1. 19E-02	1. 17E-02	1. 13E-02	1. 06E-02	9. 70E-03	8. 17E-03	5. 76E-03	3. 10E-03	6. 98E-04
94	KET	1. 80E-04	1. 79E-04	1. 76E-04	1. 69E-04	1. 60E-04	1. 46E-04	1. 23E-04	8. 65E-05	4. 66E-05	1. 05E-05
138	BZA	2. 40E-03	2. 38E-03	2. 34E-03	2. 26E-03	2. 13E-03	1. 94E-03	1. 63E-03	1. 15E-03	6. 21E-04	1. 40E-04

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EXAMPLE 1 - TEST RUN USING EKMA/CBM-X

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

         TEST CITY

LATITUDE       39.933
LONGITUDE      75.100
TIME ZONE      5.0
DATE           6      24     1980
TIME           800    TO     1800     LOCAL DAYLIGHT TIME

DILUTION DETERMINED FROM THE FOLLOWING
INVERSION HEIGHTS        INITIAL   250.      FINAL       1235.
TIMING                   START     800.      STOP        1600.

MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)
TIME        800     900     1000    1100    1200    1300    1400    1500    1600
HEIGHT      250.0   413.6   619.2   811.8   954.3   1055.0  1129.0  1186.6  1235.0

REACTIVITY
EMISSIONS        ETH  FRACTION 0.040   OLE  FRACTION 0.030   ALD2 FRACTION 0.030
EMISSIONS        FORM FRACTION 0.020   TOL  FRACTION 0.120   XYL  FRACTION 0.100
EMISSIONS        PAR  FRACTION 0.510   NR   FRACTION 0.150
SURFACE LAYER    ETH  FRACTION 0.050   OLE  FRACTION 0.030   ALD2 FRACTION 0.160
SURFACE LAYER    FORM FRACTION 0.100   TOL  FRACTION 0.070   XYL  FRACTION 0.060
SURFACE LAYER    PAR  FRACTION 0.530   NR   FRACTION 0.000
ALOFT            ETH  FRACTION 0.060   OLE  FRACTION 0.030   ALD2 FRACTION 0.090
ALOFT            FORM FRACTION 0.060   TOL  FRACTION 0.080   XYL  FRACTION 0.070
ALOFT            PAR  FRACTION 0.610   NR   FRACTION 0.000
NO2/NOX       0.250
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TRANSPORTED CONCENTRATIONS

SURFACE LAYER         OZONE   0.010      HYDROCARBON  0.038    NOX      0.000 PPM

ALOFT                 OZONE   0.070      HYDROCARBON  0.040    NOX      0.000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES     HOUR            1      2      3      4      5      6      7      8

  VOC     FRACTION      0.170  0.170  0.170  0.100  0.020  0.020  0.020  0.020

  NOX     FRACTION      0.350  0.350  0.350  0.190  0.030  0.030  0.030  0.070
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                                   EXAMPLE 1 - TEST RUN USING EKMA/CBM-X

THE ERROR TOLERANCE IS  3. 000E-03

THE TEMPERATURE USED IS  3. 030E 02

THE MIXING HEIGHT IS  2. 50E 02

THE RATE CONSTANTS USED WERE

   3. 601E-01   4. 274E 06   2. 879E 01   1. 380E 04   2. 244E 03   3. 050E 03   5. 429E-02   3. 273E-04   1. 513E-02   4. 266E 10

   6. 520E 09   1. 053E 02   3. 098E 00   2. 771E 04   6. 316E-01   1. 786E 03   3. 800E-02   5. 686E 00   3. 200E-07   1. 500E-05

   6. 482E-02   1. 580E 04   9. 542E 03   1. 214E 04   1. 414E-04   5. 042E-04   2. 546E 03   9. 770E 03   1. 839E 02   9. 363E 00

   1. 657E 00   3. 888E 03   3. 162E 03   1. 575E 03   9. 117E 00   4. 000E 02   1. 480E 01   1. 500E 04   5. 803E-04   1. 075E-03

   2. 582E 02   9. 300E-01   1. 040E 04   9. 000E 01   6. 717E 02   2. 367E 04   3. 700E 00   9. 472E-05   5. 000E 00   1. 627E 04

   8. 876E 03   4. 820E-02   5. 761E 03   1. 636E 02   1. 089E 04   4. 391E 04   1. 920E 03   2. 220E 04   4. 044E 05   2. 265E 03

   2. 415E 03   1. 080E-01   1. 729E 02   3. 240E 02   4. 400E 03   3. 700E 03   8. 282E 03   9. 600E 03   1. 441E-05   5. 800E 02

   1. 200E 04   1. 873E-03   5. 762E-04   2. 521E-04   1. 500E 04   7. 203E-03   2. 600E 04   1. 200E 04   2. 100E 01   1. 500E 02

   1. 000E 03   1. 200E 04   1. 200E 04   1. 000E 03   2. 200E 04   1. 500E 05   1. 326E 05   2. 400E 05   1. 000E 04   3. 000E 03

   7. 000E 03   1. 000E 04   1. 200E 04   1. 080E-04   3. 054E 02   8. 959E 02   4. 826E 03   4. 077E 04   5. 400E-03   5. 998E-03

   3. 999E-03   3. 999E-03   1. 140E 01   1. 129E 03   1. 175E 04   1. 170E-03   1. 990E-03   2. 500E 01   5. 800E 01   1. 000E 01

   7. 000E 00   2. 000E 02   4. 000E 02   3. 200E 02   8. 000E 01   1. 000E 04   1. 000E 03   1. 200E 02   3. 000E 01   3. 000E 01

   1. 000E 04   1. 000E 03   1. 200E 02   3. 000E 01   3. 000E 01   1. 000E 03   1. 000E 04   5. 500E 03   3. 500E 03   7. 500E 02

   1. 000E 04   1. 400E 04   2. 000E 04   2. 500E 03   3. 700E 03   1. 200E 04   4. 776E-02   1. 441E-03   2. 000E 04   1. 200E 04

   2. 000E 03   1. 200E 04   2. 000E 04   4. 000E 03   1. 000E 04   2. 400E 04   8. 800E 01   1. 000E 00
THE PHOTOLYSIS REACTIONS ARE

             1            8            9           21           26           30           31           39           40

            48           62           69           72           73           74           76           94          138

THE PHOTOLYTIC RATE CONSTANTS ARE
          3. 601E-01   3. 273E-04   1. 513E-02   6. 482E-02   5. 042E-04   9. 363E 00   1. 657E 00   5. 803E-04   1. 075E-03
          9. 472E-05   1. 080E-01   1. 441E-05   1. 873E-03   5. 762E-04   2. 521E-04   7. 203E-03   1. 080E-04   1. 441E-03
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      TIME      NMOC      NMOC/      NOX        NO2         O3          NO2         PAR
     (LDT )     TOTAL      NOX       TOTAL    FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

     800.      1.13800   9.48333    0.12000    0.25000    0.01000     0.03000     0.58114

   TIME        NO2        NO         O          O3         NO3        O1D        OH         HO2        N2O5       HNO3
 INTERVAL      HNO2       H2O2       PNA        CO         FORM       FROX       FACD       ALD2       C2O3       MEO2
               PAN        MPNA       MEO        MNIT       MEN3       MEOH       PROX       AONE       ANO2       GLY
               MGLY       MGPX       PAR        RO2        RO2R       X          ROR        NTR        KET        D
               AO2        OLE        CRIG       MCRG       HOTA       HTMA       PNO2       ETH        OZD        ACAC
               DNIT       TOL        OPEN       PHEN       BO2        PHO        BZA        BZO2       PBZN       PHO2
               PROD       NPHN       XYL        XYLO       TLA        TLO2       NR

 8.000E 02   3.000E-02  9.000E-02  0.000E-01  1.000E-02  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01
 1.000E-10   0.000E-01  0.000E-01  0.000E-01  0.000E-01  2.580E-02  0.000E-01  0.000E-01  1.954E-02  0.000E-01  0.000E-01
             0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01
             0.000E-01  0.000E-01  5.811E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01
             0.000E-01  1.707E-02  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  2.295E-02  0.000E-01  0.000E-01
             0.000E-01  1.924E-02  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01
             0.000E-01  0.000E-01  1.403E-02  0.000E-01  0.000E-01  0.000E-01  1.650E-01

NET RATES    1.488E-02 -1.519E-02  1.096E-02 -2.559E-02  1.629E-05  3.273E-06  0.000E-01  3.179E-05  0.000E-01  0.000E-01
             1.728E-09  0.000E-01  0.000E-01  4.457E-05 -1.721E-04  0.000E-01  0.000E-01 -1.007E-04  0.000E-01  1.851E-06
             0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01
             0.000E-01  0.000E-01 -3.030E-03  0.000E-01  0.000E-01  3.311E-06  0.000E-01  0.000E-01  0.000E-01  0.000E-01
             0.000E-01 -9.321E-05  1.190E-06  1.024E-06  1.139E-06  6.826E-07  0.000E-01 -1.188E-04  0.000E-01  0.000E-01
             0.000E-01 -1.024E-04  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01  0.000E-01
             0.000E-01  0.000E-01 -7.458E-05  0.000E-01  0.000E-01  0.000E-01 -9.015E-04

THE REACTION RATES ARE
      1.08E-02    0.00E-01    2.59E-02    0.00E-01    0.00E-01    0.00E-01    1.63E-05    3.27E-06    1.51E-04    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    8.64E-10    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    1.15E-06    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    1.50E-05    2.77E-05
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    1.85E-06    0.00E-01    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    9.22E-07    1.02E-06
      6.83E-07    6.83E-07    0.00E-01    0.00E-01    0.00E-01    2.69E-07    4.57E-07    0.00E-01    0.00E-01    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
      0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    1.65E-01
THE PHOTOLYTIC RATE CONSTANTS ARE
          3.601E-01   3.273E-04   1.513E-02   6.482E-02   5.042E-04   9.363E 00   1.657E 00   5.803E-04   1.075E-03
          9.472E-05   1.080E-01   1.441E-05   1.873E-03   5.762E-04   2.521E-04   7.203E-03   1.080E-04   1.441E-03

THE CURRENT MIXING HEIGHT IS      250.00

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        64.62
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         TIME       NMOC       NMOC/        NOX         NO2          O3          NO2          PAR
        (LDT )      TOTAL       NOX        TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

         900.      0.80071    8.36024     0.09578     0.51933     0.01751     0.04974     0.41364

  TIME         NO2         NO          O           O3          NO3         O1D         OH          HO2         N2O5        HNO3
INTERVAL       HNO2        H2O2        PNA         CO          FORM        FROX        FACD        ALD2        C2O3        MEO2
               PAN         MPNA        MEO         MNIT        MEN3        MEOH        PROX        AONE        ANO2        GLY
               MGLY        MGPX        PAR         RO2         RO2R        X           ROR         NTR         KET         D
               AO2         OLE         CRIG        MCRG        HOTA        HTMA        PNO2        ETH         OZD         ACAC
               DNIT        TOL         OPEN        PHEN        BO2         PHO         BZA         BZO2        PBZN        PHO2
               PROD        NPHN        XYL         XYLO        TLA         TLO2        NR

 9.000E 02   4.974E-02   4.604E-02   5.484E-09   1.751E-02   3.722E-08   3.183E-16   7.687E-08   4.309E-07   5.730E-07   1.850E-03
 2.000E 01   3.913E-04   2.865E-08   3.687E-06   3.695E-03   1.971E-02   2.216E-10   1.447E-05   1.529E-02   4.499E-08   1.735E-07
             2.422E-04   3.033E-07   2.146E-10   3.299E-06   7.883E-06   2.144E-10   1.758E-08   1.071E-03   8.677E-11   9.966E-04
             1.220E-03   4.431E-09   4.136E-01   2.017E-08   5.320E-08   2.714E-08   5.616E-11   9.565E-05   3.198E-04   5.045E-09
             2.647E-08   1.077E-02   2.136E-09   1.793E-09   1.311E-08   7.526E-10   9.032E-12   1.605E-02   1.349E-07   6.507E-06
             1.102E-08   1.339E-02   4.864E-08   4.132E-04   1.399E-09   3.340E-10   2.766E-05   1.827E-10   2.339E-07   5.634E-11
             1.212E-06   6.291E-06   9.056E-03   2.523E-09   5.385E-05   4.516E-10   1.170E-01

NET RATES    1.648E-04  -5.622E-04   1.907E-05   2.209E-04  -1.625E-07  -7.068E-08   6.738E-07  -2.484E-07   2.190E-08   4.621E-05
            -2.296E-06   1.061E-09   1.151E-07   6.764E-05  -6.430E-05  -3.554E-10   3.412E-07  -5.238E-05  -9.027E-08  -1.380E-07
             6.302E-06   8.380E-08  -5.224E-10  -5.231E-08   1.741E-07   8.084E-12   6.681E-10   1.968E-05  -1.978E-10   1.565E-05
             1.581E-05  -1.050E-08  -2.230E-03  -1.485E-08  -4.218E-08   9.019E-08  -1.922E-08   1.768E-06   5.866E-06   4.185E-08
            -1.928E-08  -8.888E-05  -8.691E-10  -4.597E-10   2.202E-09   1.490E-09  -5.397E-12  -9.374E-05   3.073E-09   1.644E-07
             3.298E-10  -7.871E-05  -2.415E-08   7.123E-06  -9.868E-10  -2.677E-09   4.631E-07  -1.452E-10   9.723E-09   1.876E-12
             4.194E-08   2.832E-07  -6.948E-05  -1.417E-09   8.906E-07  -3.741E-10  -6.305E-04

THE REACTION RATES ARE
      2.31E-02    2.34E-02    2.32E-02    3.76E-06    6.12E-07    7.70E-07    4.73E-05    1.56E-05    3.42E-04    1.36E-05
      2.08E-06    1.42E-07    2.34E-08    4.75E-05    1.17E-09    3.31E-06    2.18E-08    3.26E-06    7.33E-10    2.30E-12
      3.27E-05    6.04E-05    3.38E-05    2.41E-04    3.00E-07    1.86E-11    5.61E-12    2.94E-07    2.62E-08    4.50E-07
      7.95E-08    7.22E-10    5.87E-10    3.38E-05    3.36E-05    1.14E-07    1.26E-07    2.27E-05    1.91E-05    3.09E-05
      2.79E-08    6.82E-10    1.06E-07    1.99E-08    5.63E-08    2.78E-05    2.11E-09    2.68E-06    3.29E-08    3.37E-05
      1.99E-05    1.17E-05    4.97E-05    4.96E-05    8.70E-05    4.34E-07    1.90E-08    2.37E-07    8.68E-05    1.37E-09
      6.13E-10    4.60E-07    5.21E-12    9.76E-12    3.44E-11    7.49E-12    6.19E-10    1.86E-10    1.99E-08    4.77E-08
      4.79E-08    2.41E-06    7.41E-07    3.24E-07    1.15E-06    1.13E-05    2.44E-06    2.45E-06    1.61E-06    4.77E-06
      3.18E-05    1.11E-05    2.94E-05    2.45E-06    6.15E-08    8.42E-06    7.45E-06    1.35E-05    1.12E-04    6.26E-06
      1.46E-05    1.61E-08    1.46E-05    4.46E-08    1.80E-08    5.29E-08    2.85E-07    3.37E-05    1.02E-06    1.13E-06
      7.54E-07    7.54E-07    4.57E-09    9.94E-08    1.45E-05    3.29E-07    5.59E-07    3.28E-07    7.60E-07    1.31E-07
      9.18E-08    1.51E-07    3.01E-07    2.41E-07    6.02E-08    9.83E-07    1.06E-07    2.56E-07    1.26E-09    9.80E-10
      8.25E-07    8.92E-08    2.15E-07    1.06E-09    8.23E-10    4.16E-10    4.16E-09    5.66E-06    3.60E-06    7.72E-07
      2.24E-05    2.15E-07    4.25E-08    2.27E-08    3.11E-08    7.73E-07    1.12E-08    5.14E-08    3.32E-07    3.11E-08
      1.39E-06    1.39E-06    8.28E-08    8.32E-08    6.96E-06    1.67E-05    6.76E-06    1.17E-01
THE PHOTOLYTIC RATE CONSTANTS ARE
          4.645E-01   8.897E-04   1.951E-02   8.361E-02   6.503E-04   1.208E 01   2.137E 00   9.704E-04   1.568E-03
          1.753E-04   1.394E-01   1.858E-05   2.416E-03   7.432E-04   3.252E-04   9.290E-03   1.394E-04   1.858E-03


THE CURRENT MIXING HEIGHT IS      413.60

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        53.19
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        TIME      NMOC       NMOC/       NOX         NO2        O3          NO2         PAR
       (LDT )     TOTAL       NOX       TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

       1000.     0.59954    7.84807    0.07639     0.67084    0.03661     0.05125     0.31437

  TIME          NO2          NO           O            O3           NO3          O1D          OH           HO2          N2O5         HNO3
 INTERVAL       HNO2         H2O2         PNA          CO           FORM         FROX         FACD         ALD2         C2O3         MEO2
                PAN          MPNA         MEO          MNIT         MEN3         MEOH         PROX         AONE         ANO2         GLY
                MGLY         MGPX         PAR          RO2          RO2R         X            ROR          NTR          KET          D
                AO2          OLE          CRIG         MCRG         HOTA         HTMA         PNO2         ETH          OZD          ACAC
                DNIT         TOL          OPEN         PHEN         BO2          PHO          BZA          BZO2         PBZN         PHO2
                PROD         NPHN         XYL          XYLO         TLA          TLO2         NR

 1.000E 03     5.125E-02    2.515E-02    6.490E-09    3.661E-02    1.399E-07    1.194E-15    1.116E-07    9.061E-07    2.212E-06    5.110E-03
 2.000E 01     2.861E-04    1.840E-07    7.967E-06    8.090E-03    1.718E-02    6.463E-10    4.220E-05    1.296E-02    1.076E-07    3.513E-07
               7.242E-04    6.306E-07    2.405E-10    1.760E-06    1.809E-05    1.344E-09    1.165E-07    2.195E-03    4.472E-10    1.708E-03
               1.773E-03    1.659E-08    3.144E-01    4.025E-08    1.060E-07    3.750E-08    6.215E-11    1.972E-04    6.538E-04    7.316E-09
               5.266E-08    6.662E-03    4.306E-09    3.459E-09    1.834E-08    9.753E-10    3.798E-11    1.179E-02    3.764E-07    2.057E-05
               4.290E-08    9.848E-03    8.602E-08    7.636E-04    2.702E-09    1.757E-09    5.071E-05    7.947E-10    1.357E-06    2.450E-10
               4.871E-06    5.508E-05    5.869E-03    4.322E-09    9.651E-05    2.062E-09    8.928E-02

NET RATES     -1.813E-04   -7.754E-05    2.532E-05    4.400E-04    1.647E-06   -1.394E-07   -2.780E-06    2.534E-06    1.256E-07    6.333E-05
              -2.168E-06    4.570E-09    4.652E-07    7.966E-05   -2.217E-05    3.227E-09    5.776E-07   -2.727E-05    1.718E-07   -2.180E-07
               9.999E-06    5.326E-07   -1.283E-06   -2.202E-08    1.676E-07    3.247E-11    2.920E-09    1.831E-05    7.190E-09    8.519E-06
               3.655E-06    1.390E-07   -1.147E-03    1.592E-07    4.531E-07   -1.145E-07   -5.735E-07    1.639E-06    5.507E-06    1.103E-07
               2.073E-07   -5.042E-05   -1.621E-09   -2.224E-09   -8.768E-11    8.006E-11    1.162E-10   -5.110E-05    4.912E-09    2.998E-07
               7.146E-10   -4.178E-05    1.407E-07    4.625E-06    9.196E-09   -2.404E-08    3.113E-07    2.277E-09    2.940E-08    4.363E-12
               7.921E-08    1.492E-06   -3.879E-05    6.096E-09    5.479E-07    8.090E-09   -3.116E-04

THE REACTION RATES ARE
        2.69E-02     2.77E-02     2.65E-02     4.59E-06     7.46E-07     4.98E-07     1.02E-04     5.86E-05     8.07E-04     5.09E-05
        7.78E-06     4.31E-07     1.03E-07     9.75E-05     4.53E-09     1.28E-05     8.41E-08     1.26E-05     4.12E-10     1.23E-12
        2.70E-05     9.04E-05     2.68E-05     2.77E-04     8.94E-08     1.35E-10     5.23E-11     3.12E-07     1.05E-07     1.91E-06
        3.38E-07     3.19E-09     2.60E-09     7.31E-05     7.26E-05     3.61E-07     2.30E-07     2.88E-05     2.22E-05     3.28E-05
        2.88E-08     2.24E-09     1.69E-07     5.82E-08     5.65E-08     3.42E-05     6.71E-09     3.46E-06     5.87E-08     4.40E-05
        4.90E-05     3.49E-05     1.04E-04     1.03E-04     9.62E-05     2.66E-07     1.16E-08     2.74E-07     9.72E-05     4.57E-09
        4.74E-10     2.77E-07     2.13E-11     4.00E-11     1.66E-10     4.29E-11     2.64E-09     9.36E-10     4.61E-08     1.42E-07
        1.35E-07     4.66E-06     1.43E-06     6.28E-07     2.86E-06     1.86E-05     5.15E-06     5.01E-06     2.34E-06     5.26E-06
        3.51E-05     1.21E-05     3.20E-05     2.66E-06     7.01E-08     9.32E-06     8.24E-06     1.49E-05     1.18E-04     6.90E-06
        1.61E-05     4.78E-08     1.59E-05     1.03E-07     1.32E-08     3.87E-08     2.09E-07     3.03E-05     1.32E-06     1.46E-06
        9.75E-07     9.75E-07     1.06E-08     8.64E-08     1.55E-05     5.05E-07     8.59E-07     4.59E-07     1.06E-06     1.83E-07
        1.28E-07     1.95E-07     3.90E-07     3.12E-07     7.80E-08     1.08E-06     2.21E-07     5.17E-07     2.22E-09     1.67E-09
        8.70E-07     1.77E-07     4.15E-07     1.78E-09     1.35E-09     9.55E-10     9.55E-09     6.05E-06     3.85E-06     8.24E-07
        2.16E-05     1.50E-06     1.13E-07     1.02E-07     7.39E-08     8.15E-07     6.48E-08     1.07E-07     1.80E-06     7.39E-08
        1.31E-06     1.30E-06     2.15E-07     2.07E-07     6.55E-06     1.57E-05     9.82E-06     8.93E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
            5.250E-01    1.600E-03    2.205E-02    9.451E-02    7.351E-04    1.365E 01    2.415E 00    1.293E-03    1.909E-03
            2.671E-04    1.575E-01    2.100E-05    2.730E-03    8.401E-04    3.675E-04    1.050E-02    1.575E-04    2.100E-03


THE CURRENT MIXING HEIGHT IS      619.16

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        41.73
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      TIME      NMOC        NMOC/       NOX         NO2         O3          NO2         PAR
     (LDT )     TOTAL       NOX         TOTAL       FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

     1100.      0.49625     7.75381     0.06400     0.75461     0.05677     0.04830     0.26447

TIME          NO2          NO           O            O3           NO3          O1D          OH           HO2          N2O5         HNO3
INTERVAL      HNO2         H2O2         PNA          CO           FORM         FROX         FACD         ALD2         C2O3         MEO2
              PAN          MPNA         MEO          MNIT         MEN3         MEOH         PROX         AONE         ANO2         GLY
              MGLY         MGPX         PAR          RO2          RO2R         X            ROR          NTR          KET          D
              AO2          OLE          CRIG         MCRG         HOTA         HTMA         PNO2         ETH          OZD          ACAC
              DNIT         TOL          OPEN         PHEN         BO2          PHO          BZA          BZO2         PBZN         PHO2
              PROD         NPHN         XYL          XYLO         TLA          TLO2         NR

 1.100E 03    4.830E-02    1.571E-02    6.709E-09    5.677E-02    3.096E-07    2.597E-15    1.512E-07    1.597E-06    4.695E-06    9.558E-03
 2.000E 01    2.233E-04    7.153E-07    1.341E-05    1.353E-02    1.654E-02    1.492E-09    8.386E-05    1.177E-02    2.004E-07    5.903E-07
              1.412E-03    1.011E-06    2.588E-10    1.081E-06    2.814E-05    4.937E-09    4.552E-07    3.426E-03    1.460E-09    2.163E-03
              1.907E-03    3.777E-08    2.645E-01    7.166E-08    1.884E-07    4.750E-08    7.092E-11    3.091E-04    1.018E-03    9.896E-09
              9.348E-08    4.263E-03    5.911E-09    4.456E-09    2.086E-08    1.002E-09    8.615E-11    9.431E-03    7.124E-07    4.124E-05
              9.661E-08    7.963E-03    1.317E-07    9.866E-04    4.625E-09    4.854E-09    6.932E-05    2.173E-09    3.964E-06    6.700E-10
              1.073E-05    2.138E-04    4.028E-03    6.323E-09    1.256E-04    5.691E-09    7.635E-02

NET RATES    -1.104E-03    8.918E-04   -6.449E-05    1.418E-03    5.941E-06    1.145E-06   -1.101E-05    1.157E-05   -1.891E-07    8.673E-05
             -1.037E-06    1.466E-08   -8.256E-07    1.040E-04   -3.609E-06    1.307E-08    8.087E-07   -1.717E-05    2.318E-06    2.605E-06
              1.298E-05   -1.245E-06   -3.950E-06   -8.079E-09    1.704E-07    9.581E-11    9.301E-09    2.240E-05    2.539E-08    5.800E-06
             -2.343E-07    3.810E-07   -6.362E-04    5.431E-07    1.537E-06   -5.771E-07   -1.637E-06    1.977E-06    6.844E-06    1.552E-07
              7.019E-07   -3.281E-05    5.363E-09   -1.802E-09   -5.272E-08   -3.434E-08    1.622E-10   -3.229E-05    6.339E-09    3.920E-07
              1.019E-09   -2.511E-05    5.526E-07    2.616E-06    3.159E-08    7.154E-08    2.662E-07    1.032E-08    5.933E-08    9.123E-12
              1.188E-07    3.948E-06   -2.546E-05    2.673E-08    3.769E-07    2.245E-08   -1.539E-04

THE REACTION RATES ARE
        2.72E-02     2.87E-02     2.57E-02     4.47E-06     7.27E-07     3.21E-07     1.49E-04     1.29E-04     1.34E-03     1.11E-04
        1.69E-05     9.05E-07     2.81E-07     1.35E-04     9.44E-09     2.67E-05     1.78E-07     2.67E-05     2.43E-10     7.48E-13
        2.26E-05     1.15E-04     2.27E-05     3.04E-04     3.49E-08     5.63E-10     2.75E-10     3.30E-07     2.66E-07     4.53E-06
        8.01E-07     9.91E-09     8.06E-09     1.21E-04     1.22E-04     8.19E-07     3.91E-07     3.75E-05     2.53E-05     3.54E-05
        2.87E-08     4.76E-09     2.44E-07     1.34E-07     5.30E-08     4.21E-05     1.35E-08     3.93E-06     9.40E-08     5.12E-05
        8.59E-05     6.80E-05     1.64E-04     1.65E-04     1.01E-04     1.78E-07     7.80E-09     2.77E-07     1.05E-04     9.64E-09
        3.95E-10     1.82E-07     6.02E-11     1.13E-10     5.20E-10     1.49E-10     7.80E-09     3.07E-09     7.71E-08     3.01E-07
        2.75E-07     6.32E-06     1.95E-06     8.51E-07     4.91E-06     2.14E-05     7.50E-06     7.12E-06     3.18E-06     6.00E-06
        4.00E-05     1.35E-05     3.55E-05     2.96E-06     7.54E-08     1.06E-05     9.41E-06     1.70E-05     1.26E-04     7.85E-06
        1.83E-05     1.01E-07     1.76E-05     1.72E-07     8.74E-09     2.56E-08     1.38E-07     2.63E-05     1.31E-06     1.45E-06
        9.68E-07     9.68E-07     1.50E-08     7.14E-08     1.68E-05     6.27E-07     1.07E-06     5.21E-07     1.21E-06     2.09E-07
        1.46E-07     2.00E-07     4.01E-07     3.21E-07     8.02E-08     9.28E-07     2.85E-07     7.09E-07     2.93E-09     2.09E-09
        7.00E-07     2.15E-07     5.35E-07     2.21E-09     1.57E-09     1.35E-09     1.35E-08     6.62E-06     4.22E-06     9.03E-07
        2.07E-05     4.28E-06     2.10E-07     2.62E-07     1.26E-07     8.72E-07     1.89E-07     1.56E-07     4.69E-06     1.26E-07
        1.22E-06     1.19E-06     3.80E-07     3.57E-07     6.09E-06     1.46E-05     1.33E-05     7.64E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
           5.623E-01    2.270E-03    2.361E-02    1.012E-01    7.872E-04    1.462E 01    2.586E 00    1.527E-03    2.141E-03
           3.341E-04    1.687E-01    2.249E-05    2.924E-03    8.996E-04    3.936E-04    1.125E-02    1.687E-04    2.249E-03


THE CURRENT MIXING HEIGHT IS      811.78

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        30.69
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   TIME      NMOC       NMOC/       NOX        NO2        O3         NO2        PAR
  (LDT )     TOTAL       NOX       TOTAL     FRACTION  (INSTANT)  (INSTANT)  (INSTANT)

  1200.     0.42788    8.48858    0.05041    0.80811    0.08297    0.04073    0.23250

 TIME         NO2         NO          O           O3          NO3         O1D         OH          HO2         N2O5        HNO3
INTERVAL      HNO2        H2O2        PNA         CO          FORM        FROX        FACD        ALD2        C2O3        MEO2
              PAN         MPNA        MEO         MNIT        MEN3        MEOH        PROX        AONE        ANO2        GLY
              MGLY        MGPX        PAR         RO2         RO2R        X           ROR         NTR         KET         D
              AO2         OLE         CRIG        MCRG        HOTA        HTMA        PNO2        ETH         OZD         ACAC
              DNIT        TOL         OPEN        PHEN        BO2         PHO         BZA         BZO2        PBZN        PHO2
              PROD        NPHN        XYL         XYLO        TLA         TLO2        NR

 1.200E 03  4.073E-02   9.672E-03   6.086E-09   8.297E-02   6.154E-07   4.670E-15   2.177E-07   3.156E-06   7.848E-06   1.597E-02
 2.000E 01  1.900E-04   3.085E-06   2.234E-05   2.112E-02   1.654E-02   4.033E-09   1.454E-04   1.073E-02   4.022E-07   1.091E-06
            2.500E-03   1.574E-06   2.845E-10   7.182E-07   3.813E-05   1.914E-08   1.928E-06   5.201E-03   5.547E-09   2.516E-03
            1.890E-03   9.164E-08   2.325E-01   1.522E-07   3.999E-07   6.286E-08   8.926E-11   4.711E-04   1.540E-03   1.421E-08
            1.979E-07   2.547E-03   7.288E-09   4.901E-09   2.104E-08   8.420E-10   1.675E-10   7.648E-03   1.147E-06   6.728E-05
            1.697E-07   6.616E-03   2.243E-07   1.037E-03   9.260E-09   1.202E-08   8.810E-05   6.313E-09   1.035E-05   1.946E-09
            1.969E-05   6.291E-04   2.648E-03   9.921E-09   1.440E-04   1.609E-08   6.951E-02

NET RATES  -1.018E-04  -1.487E-04   6.956E-06   4.198E-04   7.639E-08   3.022E-07  -1.329E-06   2.840E-06  -1.785E-07   1.159E-04
           -6.622E-07   5.957E-08  -1.217E-06   1.379E-04  -1.897E-06   3.734E-09   1.125E-06  -2.021E-05   1.079E-06   1.683E-06
            1.974E-05  -1.497E-06  -3.596E-07  -6.793E-09   1.592E-07   3.460E-10   3.669E-08   3.280E-05   1.310E-08   5.158E-06
           -1.150E-06   6.049E-08  -5.426E-04   1.202E-07   3.414E-07  -6.578E-08  -3.144E-07   2.985E-06   9.699E-06   1.884E-09
            1.548E-07  -2.764E-05   1.159E-09   1.542E-09   3.129E-09   2.840E-09   4.442E-11  -3.073E-05   7.586E-09   4.482E-07
            1.267E-09  -2.316E-05   5.919E-08  -2.867E-07   5.577E-09  -3.546E-09   3.023E-07   9.232E-09   1.270E-07   2.737E-11
            1.648E-07   8.481E-06  -2.285E-05   1.499E-09   2.251E-07   4.554E-09  -1.123E-04

THE REACTION RATES ARE
      2.38E-02    2.60E-02    2.31E-02    3.42E-06    5.56E-07    1.80E-07    1.83E-04    2.30E-04    2.03E-03    1.99E-04
      3.05E-05    1.90E-06    8.11E-07    1.65E-04    1.58E-08    4.48E-05    2.98E-07    4.46E-05    1.26E-10    5.41E-13
      2.00E-05    1.40E-04    2.01E-05    3.70E-04    1.32E-08    2.52E-09    1.71E-09    4.04E-07    6.39E-07    9.34E-06
      1.65E-06    3.87E-08    3.15E-08    2.02E-04    2.04E-04    1.84E-06    7.72E-07    5.40E-05    2.76E-05    3.78E-05
      2.60E-08    9.46E-09    4.06E-07    3.63E-07    4.39E-08    5.53E-05    2.44E-08    4.17E-06    1.69E-07    6.33E-05
      1.45E-04    1.20E-04    2.56E-04    2.58E-04    1.15E-04    1.21E-07    5.28E-09    2.57E-07    1.15E-04    1.88E-08
      3.78E-10    1.26E-07    2.06E-10    3.86E-10    1.93E-09    5.98E-10    2.85E-08    1.22E-08    1.21E-07    6.57E-07
      6.44E-07    7.64E-06    2.35E-06    1.03E-06    8.22E-06    2.21E-05    1.07E-05    1.06E-05    4.57E-06    7.59E-06
      5.06E-05    1.77E-05    4.64E-05    3.87E-06    8.00E-08    1.34E-05    1.18E-05    2.14E-05    1.46E-04    9.91E-06
      2.31E-05    2.19E-07    2.30E-05    2.70E-07    4.73E-09    1.39E-08    7.48E-08    2.26E-05    1.14E-06    1.27E-06
      8.45E-07    8.45E-07    1.79E-08    5.25E-08    1.96E-05    7.43E-07    1.26E-06    5.26E-07    1.22E-06    2.10E-07
      1.47E-07    1.68E-07    3.37E-07    2.69E-07    6.74E-08    7.05E-07    2.97E-07    8.75E-07    3.62E-09    2.35E-09
      4.74E-07    2.00E-07    5.88E-07    2.43E-09    1.58E-09    1.62E-09    1.62E-08    7.92E-06    5.04E-06    1.08E-06
      2.17E-05    8.94E-06    3.84E-07    6.43E-07    2.26E-07    1.07E-06    4.94E-07    2.06E-07    9.79E-06    2.26E-07
      1.15E-06    1.15E-06    6.27E-07    6.22E-07    5.76E-06    1.38E-05    1.92E-05    6.95E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
         5.837E-01   2.772E-03   2.452E-02   1.051E-01   8.172E-04   1.518E 01   2.685E 00   1.667E-03   2.283E-03
         3.883E-04   1.751E-01   2.335E-05   3.035E-03   9.339E-04   4.086E-04   1.167E-02   1.751E-04   2.335E-03


THE CURRENT MIXING HEIGHT IS      954.30

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        21.20
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     TIME      NMOC        NMOC/        NOX          NO2          O3           NO2         PAR
     (LDT )    TOTAL       NOX          TOTAL        FRACTION     (INSTANT)    (INSTANT)   (INSTANT)

     1300.     0. 36312    10. 47368    0. 03467     0. 85408     0. 11599     0. 02961    0. 20198

  TIME          NO2          NO           O            O3           NO3          O1D          OH           HO2          N205         HNO3
INTERVAL        HNO2         H2O2         PNA          CO           FORM         FROX         FACD         ALD2         C2O3         MEO2
                PAN          MPNA         MEO          MNIT         MEN3         MEOH         PROX         AONE         ANO2         GLY
                MGLY         MGPX         PAR          RO2          RO2R         X            ROR          NTR          KET          D
                AO2          OLE          CRIG         MCRG         HOTA         HTMA         PNO2         ETH          OZD          ACAC
                DNIT         TOL          OPEN         PHEN         BO2          PHO          BZA          BZO2         PBZN         PHO2
                PROD         NPHN         XYL          XYLO         TLA          TLO2         NR

 1. 300E 03   2. 961E-02   5. 059E-03   4. 832E-09   1. 160E-01   1. 113E-06   6. 970E-15   3. 265E-07   6. 814E-06   1. 034E-05   2. 375E-02
 2. 000E 01   1. 481E-04   1. 343E-05   3. 568E-05   3. 077E-02   1. 618E-02   1. 119E-08   2. 238E-04   9. 195E-03   8. 620E-07   2. 178E-06
              4. 084E-03   2. 315E-06   3. 043E-10   3. 986E-07   4. 564E-05   7. 367E-08   8. 111E-06   7. 679E-03   2. 088E-08   2. 692E-03
              1. 692E-03   2. 275E-07   2. 020E-01   3. 613E-07   9. 496E-07   8. 639E-08   1. 164E-10   6. 982E-04   2. 269E-03   2. 122E-08
              4. 683E-07   1. 219E-03   7. 715E-09   4. 164E-09   1. 896E-08   5. 524E-10   2. 827E-10   5. 831E-03   1. 585E-06   9. 202E-05
              2. 397E-07   5. 253E-03   4. 070E-07   8. 628E-04   2. 039E-08   2. 506E-08   1. 038E-04   1. 851E-08   2. 350E-05   5. 707E-09
              3. 116E-05   1. 335E-03   1. 456E-03   1. 580E-08   1. 422E-04   4. 377E-08   6. 406E-02

NET RATES     1. 016E-04  -3. 323E-04   3. 618E-06   2. 802E-04  -1. 113E-06   7. 555E-07  -1. 539E-05   2. 117E-05  -3. 657E-07   1. 337E-04
             -6. 349E-07   2. 871E-07  -7. 536E-06   1. 725E-04  -8. 302E-06   3. 532E-08   1. 347E-06  -2. 848E-05   6. 500E-06   8. 171E-06
              2. 421E-05  -7. 257E-06  -3. 228E-06  -3. 797E-09   1. 050E-07   1. 438E-09   1. 684E-07   4. 442E-05   1. 862E-07   1. 316E-06
             -4. 596E-06   5. 494E-07  -4. 699E-04   1. 221E-06   3. 488E-06  -1. 005E-06  -3. 240E-06   3. 957E-06   1. 353E-05   1. 389E-08
              1. 570E-06  -1. 855E-05   4. 718E-09   1. 140E-08   1. 529E-08   1. 305E-08  -2. 668E-10  -2. 901E-05   6. 914E-09   3. 762E-07
              1. 108E-09  -2. 167E-05   2. 467E-07  -3. 843E-06   4. 852E-08  -1. 694E-07   1. 758E-07   8. 318E-08   2. 164E-07   7. 219E-11
              2. 031E-07   1. 305E-05  -1. 750E-05  -9. 134E-09  -1. 599E-07   4. 277E-08  -7. 293E-05

THE REACTION RATES ARE
        1. 75E-02    2. 07E-02    1. 69E-02    1. 97E-06    3. 21E-07    7. 46E-08    1. 86E-04    3. 44E-04    2. 87E-03    2. 97E-04
        4. 54E-05    3. 99E-06    2. 45E-06    1. 56E-04    2. 08E-08    5. 88E-05    3. 93E-07    5. 88E-05    4. 79E-11    3. 29E-13
        1. 57E-05    1. 53E-04    1. 58E-05    4. 18E-04    3. 62E-09    1. 11E-08    1. 12E-08    4. 72E-07    1. 43E-06    1. 71E-05
        3. 02E-06    1. 81E-07    1. 47E-07    3. 18E-04    3. 25E-04    4. 02E-06    1. 63E-06    7. 92E-05    2. 78E-05    3. 77E-05
        2. 02E-08    1. 67E-08    5. 89E-07    1. 01E-06    2. 98E-08    7. 11E-05    3. 79E-08    3. 71E-06    3. 13E-07    7. 10E-05
        2. 27E-04    1. 97E-04    3. 72E-04    3. 79E-04    1. 20E-04    6. 76E-08    2. 96E-09    2. 00E-07    1. 23E-04    3. 37E-08
        3. 14E-10    7. 05E-08    8. 20E-10    1. 54E-09    8. 26E-09    2. 75E-09    1. 23E-07    5. 64E-08    1. 81E-07    1. 45E-06
        1. 27E-06    8. 26E-06    2. 54E-06    1. 11E-06    1. 32E-05    2. 00E-05    1. 44E-05    1. 38E-05    6. 86E-06    9. 89E-06
        6. 59E-05    2. 19E-05    5. 76E-05    4. 80E-06    7. 58E-08    1. 75E-05    1. 54E-05    2. 79E-05    1. 74E-04    1. 29E-05
        3. 00E-05    4. 81E-07    2. 84E-05    4. 02E-07    1. 80E-09    5. 28E-09    2. 84E-08    1. 62E-05    7. 64E-07    8. 48E-07
        5. 65E-07    5. 65E-07    1. 55E-08    3. 18E-08    2. 24E-05    7. 91E-07    1. 35E-06    4. 74E-07    1. 10E-06    1. 90E-07
        1. 33E-07    1. 10E-07    2. 21E-07    1. 77E-07    4. 42E-08    3. 90E-07    2. 28E-07    9. 26E-07    3. 74E-09    2. 13E-09
        2. 11E-07    1. 23E-07    5. 00E-07    2. 02E-09    1. 15E-09    1. 43E-09    1. 43E-08    9. 43E-06    6. 00E-06    1. 29E-06
        2. 06E-05    1. 34E-05    6. 78E-07    1. 37E-06    3. 47E-07    1. 24E-06    1. 12E-06    2. 45E-07    1. 48E-05    3. 46E-07
        9. 50E-07    9. 59E-07    9. 29E-07    8. 86E-07    4. 75E-06    1. 14E-05    2. 87E-05    6. 41E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
           5. 900E-01   2. 962E-03   2. 478E-02   1. 062E-01   8. 260E-04   1. 534E 01   2. 714E 00   1. 718E-03   2. 328E-03
           4. 031E-04   1. 770E-01   2. 360E-05   3. 068E-03   9. 439E-04   4. 130E-04   1. 180E-02   1. 770E-04   2. 360E-03


THE CURRENT MIXING HEIGHT IS      1055. 00

THE CURRENT TEMPERATURE IS         303. 00

THE CURRENT ZENITH ANGLE IS         16. 54
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       TIME      NMOC        NMOC/        NOX         NO2          O3          NO2         PAR
      (LDT )     TOTAL        NOX        TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

      1400.     0.30728    15.20715     0.02021     0.89250     0.15395     0.01803     0.17465


   TIME        NO2         NO          O           O3          NO3         O1D         OH          HO2         N2O5        HNO3
 INTERVAL      HNO2        H2O2        PNA         CO          FORM        FROX        FACD        ALD2        C2O3        MEO2
               PAN         MPNA        MEO         MNIT        MEN3        MEOH        PROX        AONE        ANO2        GLY
               MOLY        MOPX        PAR         RO2         RO2R        X           ROR         NTR         KET         D
               AO2         OLE         CRIG        MCRG        HOTA        HTMA        PNO2        ETH         OZD         ACAC
               DNIT        TOL         OPEN        PHEN        BO2         PHO         BZA         BZO2        PBZN        PHO2
               PROD        NPHN        XYL         XYLO        TLA         TLO2        NR

 1.400E 03   1.803E-02   2.172E-03   3.447E-09   1.539E-01   1.784E-06   8.777E-15   4.919E-07   1.866E-05   1.002E-05   3.164E-02
 1.000E 01   9.942E-05   7.705E-05   5.797E-05   4.224E-02   1.510E-02   3.707E-08   3.118E-04   7.323E-03   2.160E-06   5.197E-06
             6.204E-03   3.293E-06   3.024E-10   1.792E-07   4.912E-05   3.343E-07   4.215E-05   1.099E-02   1.210E-07   2.599E-03
             1.313E-03   6.469E-07   1.747E-01   1.159E-06   3.056E-06   1.220E-07   1.515E-10   1.005E-03   3.243E-03   3.173E-08
             1.495E-06   4.509E-04   6.982E-09   2.586E-09   1.546E-08   2.769E-10   3.829E-10   4.146E-03   1.924E-06   1.089E-04
             2.865E-07   3.975E-03   8.457E-07   5.741E-04   5.647E-08   4.433E-08   1.106E-04   6.397E-08   4.818E-05   1.971E-08
             4.402E-05   2.176E-03   6.421E-04   2.423E-08   1.156E-04   1.313E-07   6.073E-02

NET RATES   -1.692E-04  -6.101E-05   4.810E-07   6.374E-04  -2.862E-07   2.392E-07   2.086E-06  -2.849E-06   5.609E-08   1.223E-04
            -8.455E-07   2.222E-06   1.530E-06   2.013E-04  -2.708E-05  -3.813E-09   1.486E-06  -3.281E-05  -9.138E-07  -1.164E-06
             4.075E-05   1.104E-06   5.869E-07  -2.989E-09   1.955E-08   8.433E-09   1.150E-06   6.145E-05  -1.861E-08  -3.931E-06
            -7.458E-06  -6.742E-08  -4.536E-04  -1.344E-07  -3.884E-07   1.678E-07   4.352E-07   5.748E-06   1.803E-05  -1.736E-08
            -1.729E-07  -9.048E-06   1.646E-09   1.496E-09   1.449E-09   7.272E-10   1.942E-11  -2.718E-05   4.602E-09   2.066E-07
             5.586E-10  -2.102E-05  -3.853E-08  -4.881E-06  -5.676E-09   1.134E-09   1.935E-08  -8.717E-09   5.369E-07   3.744E-10
             2.169E-07   1.391E-05  -1.063E-05   1.146E-10  -6.159E-07  -3.589E-09  -4.571E-05


THE REACTION RATES ARE
     1.05E-02      1.47E-02      9.63E-03      8.58E-07      1.39E-07      2.28E-08      1.51E-04      4.32E-04      3.78E-03      3.74E-04
     5.72E-05      7.98E-06      8.90E-06      1.07E-04      2.03E-08      5.74E-05      3.81E-07      5.70E-05      1.25E-11      1.48E-13
     1.05E-05      1.40E-04      1.02E-05      4.92E-04      6.67E-10      6.31E-08      9.65E-08      4.78E-07      2.86E-06      2.71E-05
     4.80E-06      1.35E-06      1.10E-06      5.30E-04      5.29E-04      8.31E-06      4.17E-06      1.11E-04      2.53E-05      3.46E-05
     1.34E-08      2.50E-08      8.37E-07      3.34E-06      1.70E-08      8.53E-05      4.83E-08      2.87E-06      6.83E-07      7.63E-05
     3.46E-04      2.99E-04      5.40E-04      5.39E-04      1.23E-04      2.88E-08      1.26E-09      1.21E-07      1.22E-04      5.47E-08
     2.13E-10      3.15E-08      4.67E-09      8.75E-09      4.94E-08      1.73E-08      8.03E-07      3.87E-07      2.57E-07      3.13E-06
     3.15E-06      7.90E-06      2.43E-06      1.06E-06      1.92E-05      1.54E-05      1.68E-05      1.69E-05      1.03E-05      1.29E-05
     8.59E-05      3.02E-05      7.97E-05      6.64E-06      6.01E-08      2.27E-05      2.01E-05      3.64E-05      2.13E-04      1.66E-05
     3.88E-05      1.03E-06      3.90E-05      5.69E-07      4.75E-10      1.39E-09      7.50E-09      9.04E-06      3.75E-07      4.16E-07
     2.78E-07      2.78E-07      9.17E-09      1.61E-08      2.40E-05      7.47E-07      1.27E-06      3.86E-07      8.97E-07      1.55E-07
     1.08E-07      5.54E-08      1.11E-07      8.86E-08      2.21E-08      1.52E-07      1.26E-07      8.38E-07      3.16E-09      1.53E-09
     5.62E-08      4.66E-08      3.10E-07      1.17E-09      5.68E-10      8.32E-10      8.32E-09      1.08E-05      6.84E-06      1.47E-06
     1.84E-05      1.43E-05      1.09E-06      2.88E-06      5.14E-07      1.47E-06      2.30E-06      2.59E-07      1.60E-05      5.14E-07
     6.32E-07      6.31E-07      1.14E-06      1.14E-06      3.16E-06      7.58E-06      4.33E-05      6.07E-02
THE PHOTOLYTIC RATE CONSTANTS ARE
          5.849E-01   2.806E-03   2.457E-02   1.053E-01   8.188E-04   1.521E 01   2.690E 00   1.676E-03   2.292E-03
          3.915E-04   1.755E-01   2.340E-05   3.041E-03   9.358E-04   4.094E-04   1.170E-02   1.755E-04   2.340E-03


THE CURRENT MIXING HEIGHT IS     1128.96

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        20.46
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  TIME      NMOC       NMOC/        NOX         NO2         O3          NO2         PAR
 (LDT )     TOTAL       NOX        TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

 1500.     0. 25729   28. 01425    0. 00918    0. 92140    0. 19197    0. 00846    0. 14779

  TIME        NO2         NO          O           O3          NO3         O1D         OH          HO2         N2O5        HNO3
 INTERVAL     HNO2        H2O2        PNA         CO          FORM        FROX        FACD        ALD2        C2O3        MEO2
              PAN         MPNA        MEO         MNIT        MEN3        MEOH        PROX        AONE        ANO2        GLY
              MGLY        MGPX        PAR         RO2         RO2R        X           ROR         NTR         KET         D
              AO2         OLE         CRIG        MCRG        HOTA        HTMA        PNO2        ETH         OZD         ACAC
              DNIT        TOL         OPEN        PHEN        BO2         PHO         BZA         BZO2        PBZN        PHO2
              PROD        NPHN        XYL         XYLO        TLA         TLO2        NR

 1. 500E 03  8. 463E-03  7. 219E-04  2. 283E-09  1. 920E-01  2. 198E-06  9. 086E-15  6. 222E-07  4. 924E-05  5. 798E-06  3. 714E-02
 5. 000E 00  4. 668E-05  5. 725E-04  7. 158E-05  5. 420E-02  1. 293E-02  9. 667E-08  3. 932E-04  5. 452E-03  5. 993E-06  1. 338E-05
             8. 520E-03  3. 971E-06  2. 587E-10  5. 570E-08  4. 756E-05  2. 110E-06  2. 962E-04  1. 490E-02  6. 250E-07  2. 184E-03
             8. 462E-04  1. 594E-06  1. 478E-01  3. 739E-06  9. 877E-06  1. 495E-07  1. 620E-10  1. 376E-03  4. 394E-03  3. 968E-08
             4. 777E-06  1. 443E-04  5. 525E-09  1. 214E-09  1. 137E-08  1. 104E-10  4. 552E-10  2. 689E-03  2. 114E-06  1. 158E-04
             3. 032E-07  2. 802E-03  1. 821E-06  3. 384E-04  1. 521E-07  7. 057E-08  1. 016E-04  2. 241E-07  8. 510E-05  6. 895E-08
             5. 628E-05  2. 891E-03  2. 329E-04  3. 354E-08  7. 339E-05  3. 182E-07  5. 853E-02

 NET RATES  -1. 034E-04 -3. 859E-05 -1. 104E-06  5. 442E-04 -1. 868E-07  1. 133E-07  4. 207E-06 -7. 184E-06  2. 684E-08  6. 283E-05
            -7. 794E-07  1. 532E-05  3. 683E-06  1. 856E-04 -4. 026E-05 -6. 075E-09  1. 182E-06 -2. 724E-05 -1. 368E-06 -2. 779E-06
             3. 327E-05  2. 592E-06  9. 694E-07 -1. 366E-09 -5. 304E-08  5. 648E-08  8. 074E-06  6. 369E-05 -3. 852E-08 -8. 491E-06
            -7. 241E-06 -1. 202E-07 -4. 249E-04 -2. 579E-07 -7. 553E-07  2. 641E-07  8. 950E-07  6. 162E-06  1. 861E-05 -4. 244E-08
            -3. 350E-07 -2. 714E-06  1. 133E-09  8. 530E-10  9. 956E-10  3. 766E-10  1. 728E-12 -2. 083E-05  2. 176E-09  6. 132E-08
             1. 079E-10 -1. 738E-05 -8. 366E-08 -3. 108E-06 -1. 060E-08 -1. 576E-08 -2. 497E-07 -1. 123E-08  6. 146E-07  1. 207E-09
             1. 886E-07  9. 839E-06 -4. 166E-06 -7. 356E-10 -6. 761E-07 -5. 869E-09 -3. 103E-05

 THE REACTION RATES ARE
       4. 78E-03    9. 76E-03    3. 99E-03    2. 67E-07    4. 34E-08    5. 03E-09    8. 82E-05    4. 47E-04    4. 56E-03    3. 88E-04
       5. 92E-05    1. 26E-05    2. 93E-05    4. 40E-05    1. 17E-08    3. 32E-05    2. 20E-07    3. 30E-05    1. 95E-12    3. 27E-14
       4. 75E-06    8. 32E-05    4. 29E-06    4. 31E-04    7. 37E-11    4. 53E-07    9. 07E-07    2. 84E-07    4. 25E-06    3. 23E-05
       5. 71E-06    9. 43E-06    7. 67E-06    6. 56E-04    6. 53E-04    1. 35E-05    9. 42E-06    1. 21E-04    2. 00E-05    2. 79E-05
       7. 62E-09    2. 64E-08    7. 26E-07    8. 70E-06    8. 36E-09    8. 03E-05    4. 43E-08    1. 85E-06    1. 34E-06    7. 04E-05
       4. 50E-04    4. 11E-04    6. 52E-04    6. 50E-04    1. 05E-04    8. 20E-09    3. 59E-10    4. 86E-08    1. 05E-04    6. 70E-08
       8. 37E-11    9. 44E-09    3. 10E-08    5. 80E-08    3. 53E-07    1. 33E-07    5. 46E-06    2. 83E-06    3. 37E-07    5. 38E-06
       5. 41E-06    6. 42E-06    1. 97E-06    8. 64E-07    2. 04E-05    9. 56E-06    1. 37E-05    1. 38E-05    1. 31E-05    1. 38E-05
       9. 19E-05    3. 24E-05    8. 56E-05    7. 13E-06    3. 02E-08    2. 43E-05    2. 15E-05    3. 89E-05    2. 21E-04    1. 76E-05
       4. 11E-05    1. 74E-06    4. 14E-05    7. 45E-07    1. 01E-10    2. 95E-10    1. 59E-09    3. 66E-06    1. 50E-07    1. 66E-07
       1. 11E-07    1. 11E-07    3. 62E-09    6. 93E-09    1. 97E-05    6. 04E-07    1. 03E-06    2. 84E-07    6. 59E-07    1. 14E-07
       7. 96E-08    2. 21E-08    4. 42E-08    3. 53E-08    8. 83E-09    3. 99E-08    4. 68E-08    6. 63E-07    2. 14E-09    9. 04E-10
       8. 76E-09    1. 03E-08    1. 46E-07    4. 71E-10    1. 99E-10    3. 29E-10    3. 29E-09    9. 59E-06    6. 10E-06    1. 31E-06
       1. 31E-05    1. 04E-05    1. 26E-06    4. 74E-06    5. 99E-07    1. 32E-06    4. 06E-06    2. 30E-07    1. 19E-05    5. 97E-07
       2. 90E-07    2. 91E-07    9. 13E-07    9. 19E-07    1. 45E-06    3. 48E-06    5. 48E-05    5. 85E-02

 THE PHOTOLYTIC RATE CONSTANTS ARE
          5. 650E-01   2. 328E-03   2. 373E-02   1. 017E-01   7. 910E-04   1. 469E 01   2. 599E 00   1. 545E-03   2. 158E-03
          3. 401E-04   1. 695E-01   2. 260E-05   2. 938E-03   9. 041E-04   3. 955E-04   1. 130E-02   1. 695E-04   2. 260E-03


 THE CURRENT MIXING HEIGHT IS    1186. 57

 THE CURRENT TEMPERATURE IS       303. 00

 THE CURRENT ZENITH ANGLE IS       29. 68
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    TIME      NMOC        NMOC/        NOX         NO2          O3          NO2         PAR
    (LDT )    TOTAL        NOX        TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

    1600.    0. 22159    44. 88364    0. 00494    0. 93669    0. 21534    0. 00462    0. 12665

   TIME          NO2          NO           O            O3           NO3          O1D          OH           HO2          N2O5         HNO3
 INTERVAL        HNO2         H2O2         PNA          CO           FORM         FROX         FACD         ALD2         C2O3         MEO2
                 PAN          MPNA         MEO          MNIT         MEN3         MEOH         PROX         AONE         ANO2         GLY
                 MGLY         MGPX         PAR          RO2          RO2R         X            ROR          NTR          KET          D
                 AO2          OLE          CRIG         MCRG         HOTA         HTMA         PNO2         ETH          OZD          ACAC
                 DNIT         TOL          OPEN         PHEN         BO2          PHO          BZA          BZO2         PBZN         PHO2
                 PROD         NPHN         XYL          XYLO         TLA          TLO2         NR

 1. 600E 03   4. 624E-03   3. 126E-04   1. 773E-09   2. 153E-01   2. 082E-06   7. 306E-15   5. 044E-07   6. 278E-05   3. 011E-06   3. 913E-02
 1. 673E 01   1. 836E-05   1. 827E-03   5. 021E-05   6. 276E-02   1. 087E-02   1. 083E-07   4. 443E-04   4. 259E-03   1. 109E-05   2. 095E-05
              9. 313E-03   3. 410E-06   1. 792E-10   1. 782E-08   4. 400E-05   8. 274E-06   1. 102E-03   1. 787E-02   1. 390E-06   1. 678E-03
              5. 159E-04   1. 804E-06   1. 266E-01   5. 991E-06   1. 570E-05   1. 207E-07   1. 126E-10   1. 669E-03   5. 262E-03   3. 182E-08
              7. 509E-06   6. 584E-05   4. 120E-09   6. 633E-10   8. 245E-09   5. 668E-11   4. 535E-10   1. 792E-03   2. 195E-06   1. 177E-04
              3. 041E-07   2. 023E-03   2. 197E-06   1. 997E-04   2. 039E-07   7. 367E-08   8. 337E-05   4. 727E-07   1. 084E-04   1. 453E-07
              6. 575E-05   3. 297E-03   1. 041E-04   2. 801E-08   4. 403E-05   3. 551E-07   5. 685E-02

 NET RATES   -5. 490E-05  -4. 804E-06  -1. 915E-09   2. 913E-04   1. 500E-08   6. 548E-11  -7. 808E-08   2. 114E-07  -4. 537E-08   1. 493E-05
             -3. 465E-07   2. 295E-05  -4. 873E-07   1. 108E-04  -3. 061E-05  -4. 384E-10   6. 270E-07  -1. 603E-05   4. 243E-08   1. 500E-07
              3. 618E-07  -1. 315E-08   2. 290E-08  -4. 043E-10  -5. 932E-08   1. 370E-07   1. 689E-05   3. 844E-05   1. 233E-08  -7. 925E-06
             -4. 422E-06  -1. 590E-09  -3. 249E-04   2. 978E-08   7. 640E-08   1. 065E-08   1. 181E-08   3. 880E-06   1. 110E-05   1. 384E-09
              3. 621E-08  -1. 298E-06  -4. 467E-11   4. 741E-12  -9. 845E-11   7. 263E-12   3. 118E-12  -1. 221E-05   8. 016E-10   6. 202E-09
             -4. 791E-11  -1. 093E-05   2. 609E-09  -1. 849E-06   4. 553E-10  -3. 798E-09  -3. 048E-07   4. 336E-09   2. 221E-07   1. 534E-09
              1. 355E-07   4. 757E-06  -1. 736E-06  -1. 106E-10  -3. 666E-07  -6. 389E-11  -3. 546E-05

 THE REACTION RATES ARE
        2. 45E-03    7. 58E-03    1. 94E-03    1. 13E-07    1. 84E-08    1. 69E-09    5. 41E-05    3. 59E-04    4. 79E-03    3. 12E-04
        4. 76E-05    1. 14E-05    4. 19E-05    1. 80E-05    6. 08E-09    1. 72E-05    1. 14E-07    1. 71E-05    4. 63E-13    5. 05E-15
        1. 75E-06    3. 69E-05    1. 50E-06    2. 38E-04    1. 38E-11    1. 35E-06    2. 35E-06    9. 05E-08    3. 63E-06    2. 87E-05
        5. 07E-06    1. 53E-05    1. 25E-05    4. 57E-04    4. 58E-04    1. 27E-05    1. 01E-05    8. 22E-05    1. 43E-05    2. 10E-05
        4. 97E-09    2. 10E-08    3. 52E-07    9. 74E-06    5. 07E-09    5. 08E-05    3. 28E-08    1. 17E-06    1. 34E-06    5. 64E-05
        4. 55E-04    4. 49E-04    5. 58E-04    5. 58E-04    7. 13E-05    2. 46E-09    1. 08E-10    1. 84E-08    7. 24E-05    5. 03E-08
        2. 17E-11    2. 83E-09    7. 59E-08    1. 42E-07    1. 02E-06    4. 55E-07    1. 09E-05    6. 68E-06    3. 78E-07    5. 23E-06
        5. 22E-06    4. 62E-06    1. 42E-06    6. 22E-07    1. 27E-05    5. 46E-06    6. 77E-06    6. 77E-06    1. 06E-05    9. 58E-06
        6. 39E-05    2. 25E-05    5. 89E-05    4. 91E-06    1. 15E-08    1. 69E-05    1. 49E-05    2. 70E-05    1. 53E-04    1. 21E-05
        2. 82E-05    1. 67E-06    2. 82E-05    8. 36E-07    3. 56E-11    1. 05E-10    5. 63E-10    1. 35E-06    7. 66E-08    8. 50E-08
        5. 67E-08    5. 67E-08    1. 56E-09    3. 59E-09    1. 06E-05    4. 52E-07    7. 68E-07    2. 06E-07    4. 78E-07    8. 25E-08
        5. 77E-08    1. 13E-08    2. 27E-08    1. 81E-08    4. 53E-09    1. 29E-08    1. 91E-08    4. 94E-07    1. 34E-09    5. 26E-10
        2. 07E-09    3. 07E-09    7. 96E-08    2. 16E-10    8. 47E-11    1. 42E-10    1. 42E-09    5. 61E-06    3. 57E-06    7. 65E-07
        6. 87E-06    5. 82E-06    8. 41E-07    5. 47E-06    5. 47E-07    7. 65E-07    5. 18E-06    1. 77E-07    6. 81E-06    5. 45E-07
        1. 05E-07    1. 05E-07    4. 44E-07    4. 44E-07    5. 25E-07    1. 26E-06    4. 44E-05    5. 68E-02
 THE PHOTOLYTIC RATE CONSTANTS ARE
          5. 293E-01   1. 669E-03   2. 223E-02   9. 528E-02   7. 411E-04   1. 376E 01   2. 435E 00   1. 319E-03   1. 935E-03
          2. 748E-04   1. 588E-01   2. 117E-05   2. 753E-03   8. 469E-04   3. 705E-04   1. 059E-02   1. 588E-04   2. 117E-03


 THE CURRENT MIXING HEIGHT IS     1235. 00

 THE CURRENT TEMPERATURE IS        303. 00

 THE CURRENT ZENITH ANGLE IS        40. 64
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     TIME      NMOC       NMOC/        NOX         NO2          O3          NO2         PAR
    (LDT )     TOTAL       NOX        TOTAL      FRACTION    (INSTANT)   (INSTANT)   (INSTANT)

    1700.     0.20272    60.87071     0.00333     0.94642     0.23147     0.00315     0.11464


  TIME          NO2         NO          O           O3          NO3         O1D         OH          HO2         N2O5        HNO3
INTERVAL        HNO2        H2O2        PNA         CO          FORM        FROX        FACD        ALD2        C2O3        MEO2
                PAN         MPNA        MEO         MNIT        MEN3        MEOH        PROX        AONE        ANO2        GLY
                MGLY        MGPX        PAR         RO2         RO2R        X           ROR         NTR         KET         D
                AO2         OLE         CRIG        MCRG        HOTA        HTMA        PNO2        ETH         OZD         ACAC
                DNIT        TOL         OPEN        PHEN        BO2         PHO         BZA         BZO2        PBZN        PHO2
                PROD        NPHN        XYL         XYLO        TLA         TLO2        NR

 1.700E 03   3.152E-03   1.784E-04   1.473E-09   2.315E-01   2.000E-06   4.494E-15   3.377E-07   5.628E-05   1.967E-06   4.063E-02
 5.000E 00   7.577E-06   3.110E-03   3.067E-05   6.966E-02   9.749E-03   8.840E-08   4.857E-04   3.645E-03   1.491E-05   2.447E-05
             8.923E-03   2.715E-06   1.221E-10   7.273E-09   4.232E-05   1.915E-05   2.288E-03   2.011E-02   1.839E-06   1.322E-03
             3.311E-04   1.363E-06   1.146E-01   6.508E-06   1.671E-05   8.123E-08   6.846E-11   1.894E-03   5.900E-03   2.116E-08
             7.940E-06   2.032E-05   3.005E-09   2.250E-10   6.159E-09   1.880E-11   2.371E-10   1.297E-03   2.291E-06   1.203E-04
             3.084E-07   1.599E-03   1.875E-06   1.159E-04   1.896E-07   6.202E-08   6.981E-05   6.995E-07   1.152E-04   2.154E-07
             7.480E-05   3.596E-03   4.503E-05   1.429E-08   2.984E-05   2.851E-07   5.685E-02

NET RATES   -1.012E-05  -1.186E-06   2.234E-07   2.043E-04   2.139E-09  -8.647E-09  -3.656E-09  -1.624E-07  -3.682E-09   1.774E-05
            -9.377E-08   1.760E-05  -2.497E-07   9.187E-05  -1.335E-05  -6.585E-10   5.678E-07  -7.525E-06  -2.160E-08  -8.613E-09
            -1.297E-05   2.910E-10   2.242E-09  -7.949E-11  -2.383E-08   1.940E-07   1.946E-05   2.911E-05   5.321E-10  -5.062E-06
            -2.322E-06  -1.102E-08  -1.593E-04  -1.398E-08  -4.222E-08   3.045E-09  -2.758E-09   2.987E-06   8.185E-06   1.724E-09
            -2.067E-08  -3.716E-07   7.671E-12   2.290E-12  -2.345E-13   3.032E-12  -2.134E-12  -6.096E-06   1.298E-09   2.700E-08
             4.230E-11  -5.267E-06  -1.008E-08  -1.203E-06  -8.365E-10   3.926E-10  -1.974E-07   1.040E-09   8.636E-09   5.813E-10
             1.318E-07   3.910E-06  -5.475E-07  -1.898E-10  -1.710E-07  -1.917E-09   0.000E-01


THE REACTION RATES ARE
      1.49E-03     6.29E-03     1.19E-03     6.40E-08     1.04E-08     8.01E-10     3.96E-05     2.21E-04     4.59E-03     1.92E-04
      2.93E-05     8.24E-06     4.04E-05     9.89E-06     3.98E-09     1.13E-05     7.48E-08     1.12E-05     1.80E-13     8.61E-16
      6.44E-07     1.68E-05     5.75E-07     1.22E-04     4.50E-12     2.06E-06     2.67E-06     2.50E-08     2.52E-06     2.45E-05
      4.34E-06     1.23E-05     1.00E-05     2.79E-04     2.80E-04     9.41E-06     8.12E-06     4.94E-05     9.82E-06     1.57E-05
      3.71E-09     1.81E-08     1.64E-07     7.96E-06     3.60E-09     2.91E-05     2.70E-08     6.72E-07     1.03E-06     4.33E-05
      4.17E-04     4.30E-04     4.44E-04     4.44E-04     4.76E-05     9.56E-10     4.18E-11     8.54E-09     4.94E-05     3.24E-08
      5.93E-12     1.03E-09     1.04E-07     1.94E-07     1.61E-06     8.22E-07     1.14E-05     8.05E-06     3.80E-07     3.94E-06
      3.94E-06     3.25E-06     9.99E-07     4.37E-07     6.70E-06     3.13E-06     2.91E-06     2.92E-06     7.09E-06     5.81E-06
      3.87E-05     1.39E-05     3.58E-05     2.98E-06     4.75E-09     1.03E-05     9.08E-06     1.64E-05     9.31E-05     7.28E-06
      1.70E-05     1.25E-06     1.70E-05     8.36E-07     9.14E-12     2.68E-11     1.44E-10     2.80E-07     2.54E-08     2.82E-08
      1.88E-08     1.88E-08     4.63E-10     2.16E-09     5.15E-06     3.51E-07     5.97E-07     1.54E-07     3.57E-07     6.16E-08
      4.31E-08     3.76E-09     7.52E-09     6.02E-09     1.50E-09     5.36E-09     9.47E-09     3.61E-07     8.79E-10     3.29E-10
      4.02E-10     7.09E-10     2.70E-08     6.58E-11     2.46E-11     4.23E-11     4.23E-10     2.97E-06     1.89E-06     4.05E-07
      3.35E-06     3.25E-06     4.72E-07     5.51E-06     4.62E-07     4.06E-07     5.50E-06     1.32E-07     3.91E-06     4.61E-07
      3.04E-08     3.06E-08     2.02E-07     2.04E-07     1.52E-07     3.65E-07     2.97E-05     5.68E-02
THE PHOTOLYTIC RATE CONSTANTS ARE
         4.720E-01    9.549E-04    1.983E-02    8.497E-02    6.609E-04    1.227E 01    2.171E 00    1.007E-03    1.607E-03
         1.843E-04    1.416E-01    1.888E-05    2.455E-03    7.553E-04    3.304E-04    9.441E-03    1.416E-04    1.888E-03


THE CURRENT MIXING HEIGHT IS     1235.00

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        52.08
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         TIME      NMOC       NMOC/        NOX          NO2          O3           NO2          PAR
        (LDT )     TOTAL      NOX          TOTAL        FRACTION    (INSTANT)    (INSTANT)    (INSTANT)

        1800.    0. 19270   60. 31772    0. 00319     0. 95684     0. 24039     0. 00306     0. 10780

   TIME          NO2          NO           O            O3           NO3          O1D          OH           HO2          N2O5         HNO3
 INTERVAL        HNO2         H2O2         PNA          CO           FORM         FROX         FACD         ALD2         C2O3         MEO2
                 PAN          MPNA         MEO          MNIT         MEN3         MEOH         PROX         AONE         ANO2         GLY
                 MGLY         MGPX         PAR          RO2          RO2R         X            ROR          NTR          KET          D
                 AO2          OLE          CRIG         MCRG         HOTA         HTMA         PNO2         ETH          OZD          ACAC
                 DNIT         TOL          OPEN         PHEN         BO2          PHO          BZA          BZO2         PBZN         PHO2
                 PROD         NPHN         XYL          XYLO         TLA          TLO2         NR

 1. 800E 03   3. 057E-03   1. 379E-04   1. 167E-09   2. 404E-01   2. 593E-06   1. 826E-15   1. 993E-07   4. 093E-05   2. 467E-06   4. 139E-02
 2. 000E 01   4. 370E-06   3. 792E-03   2. 164E-05   7. 367E-02   9. 340E-03   6. 191E-08   5. 137E-04   3. 345E-03   1. 365E-05   2. 154E-05
              8. 008E-03   2. 319E-06   8. 367E-11   4. 770E-09   4. 130E-05   2. 935E-05   3. 212E-03   2. 133E-02   1. 491E-06   1. 092E-03
              2. 366E-04   7. 474E-07   1. 078E-01   4. 813E-06   1. 202E-05   4. 859E-08   3. 813E-11   2. 022E-03   6. 237E-03   1. 245E-08
              5. 694E-06   9. 038E-06   2. 449E-09   1. 044E-10   5. 084E-09   8. 683E-12   1. 739E-10   1. 045E-03   2. 355E-06   1. 213E-04
              3. 102E-07   1. 385E-03   1. 202E-06   5. 433E-05   1. 257E-07   3. 924E-08   6. 072E-05   6. 797E-07   1. 110E-04   2. 098E-07
              8. 116E-05   3. 771E-03   2. 704E-05   6. 594E-09   2. 316E-05   1. 707E-07   5. 685E-02

 NET RATES   -5. 122E-07   2. 414E-06   1. 734E-05   1. 048E-04  -2. 019E-07  -8. 359E-07  -4. 638E-08  -6. 134E-08   3. 190E-08   1. 032E-05
             -3. 943E-08   7. 910E-06  -1. 558E-07   5. 312E-05  -3. 269E-06  -2. 629E-09   4. 182E-07  -3. 722E-06   1. 270E-07   5. 935E-08
             -1. 571E-05  -1. 250E-07  -3. 576E-08  -2. 973E-11  -1. 296E-08   1. 504E-07   1. 267E-05   1. 579E-05  -1. 413E-09  -3. 139E-06
             -1. 201E-06  -1. 084E-08  -8. 925E-05  -1. 783E-08  -5. 279E-08   1. 757E-08  -5. 378E-08   1. 659E-06   4. 247E-06   1. 288E-08
             -2. 638E-08  -1. 159E-07   4. 347E-11   5. 257E-12   6. 460E-11   4. 393E-12   3. 405E-12  -3. 242E-06   9. 717E-10   1. 252E-08
              2. 398E-11  -2. 692E-06  -1. 012E-08  -9. 521E-07  -9. 135E-10   1. 444E-08  -1. 246E-07   1. 175E-09  -1. 059E-07  -3. 902E-10
              9. 049E-08   2. 399E-06  -1. 940E-07  -1. 324E-10  -8. 141E-08  -1. 794E-09   0. 000E-01

 THE REACTION RATES ARE
        1. 14E-03    4. 99E-03    9. 54E-04    4. 92E-08    8. 00E-09    4. 91E-10    3. 99E-05    8. 90E-05    3. 76E-03    7. 79E-05
        1. 19E-05    5. 05E-06    3. 05E-05    9. 91E-06    5. 01E-09    1. 42E-05    9. 38E-08    1. 40E-05    1. 35E-13    2. 86E-16
        2. 93E-07    9. 63E-06    2. 62E-07    6. 85E-05    2. 69E-12    1. 98E-06    1. 92E-06    8. 51E-09    1. 52E-06    2. 51E-05
        4. 44E-06    6. 51E-06    5. 30E-06    1. 97E-04    1. 97E-04    5. 87E-06    5. 66E-06    2. 79E-05    5. 77E-06    1. 06E-05
        2. 81E-09    2. 25E-08    8. 88E-08    5. 57E-06    2. 62E-09    1. 58E-05    3. 21E-08    3. 40E-07    6. 85E-07    3. 06E-05
        3. 70E-04    3. 86E-04    3. 79E-04    3. 80E-04    3. 23E-05    5. 07E-10    2. 21E-11    5. 68E-09    3. 38E-05    1. 86E-08
        2. 30E-12    5. 34E-10    8. 02E-08    1. 50E-07    1. 29E-06    6. 89E-07    7. 30E-06    5. 36E-06    3. 18E-07    2. 47E-06
        2. 47E-06    2. 12E-06    6. 51E-07    2. 85E-07    3. 26E-06    1. 76E-06    1. 23E-06    1. 24E-06    4. 18E-06    3. 22E-06
        2. 15E-05    7. 96E-06    1. 99E-05    1. 66E-06    2. 56E-09    5. 72E-06    5. 06E-06    9. 15E-06    5. 24E-05    4. 03E-06
        9. 39E-06    7. 76E-07    9. 42E-06    6. 97E-07    3. 22E-12    9. 45E-12    5. 09E-11    7. 34E-08    1. 17E-08    1. 30E-08
        8. 69E-09    8. 69E-09    2. 67E-10    1. 38E-09    2. 45E-06    2. 94E-07    5. 00E-07    1. 27E-07    2. 95E-07    5. 08E-08
        3. 56E-08    1. 74E-09    3. 47E-09    2. 78E-09    6. 95E-10    3. 38E-09    7. 49E-09    2. 94E-07    6. 86E-10    2. 46E-10
        1. 44E-10    3. 19E-10    1. 25E-08    2. 92E-11    1. 05E-11    2. 40E-11    2. 40E-10    1. 52E-06    9. 66E-07    2. 07E-07
        1. 66E-06    1. 97E-06    2. 42E-07    5. 19E-06    3. 47E-07    2. 08E-07    5. 30E-06    9. 05E-08    2. 40E-06    3. 47E-07
        1. 08E-08    1. 09E-08    9. 23E-08    9. 41E-08    5. 39E-08    1. 29E-07    1. 75E-05    5. 68E-02

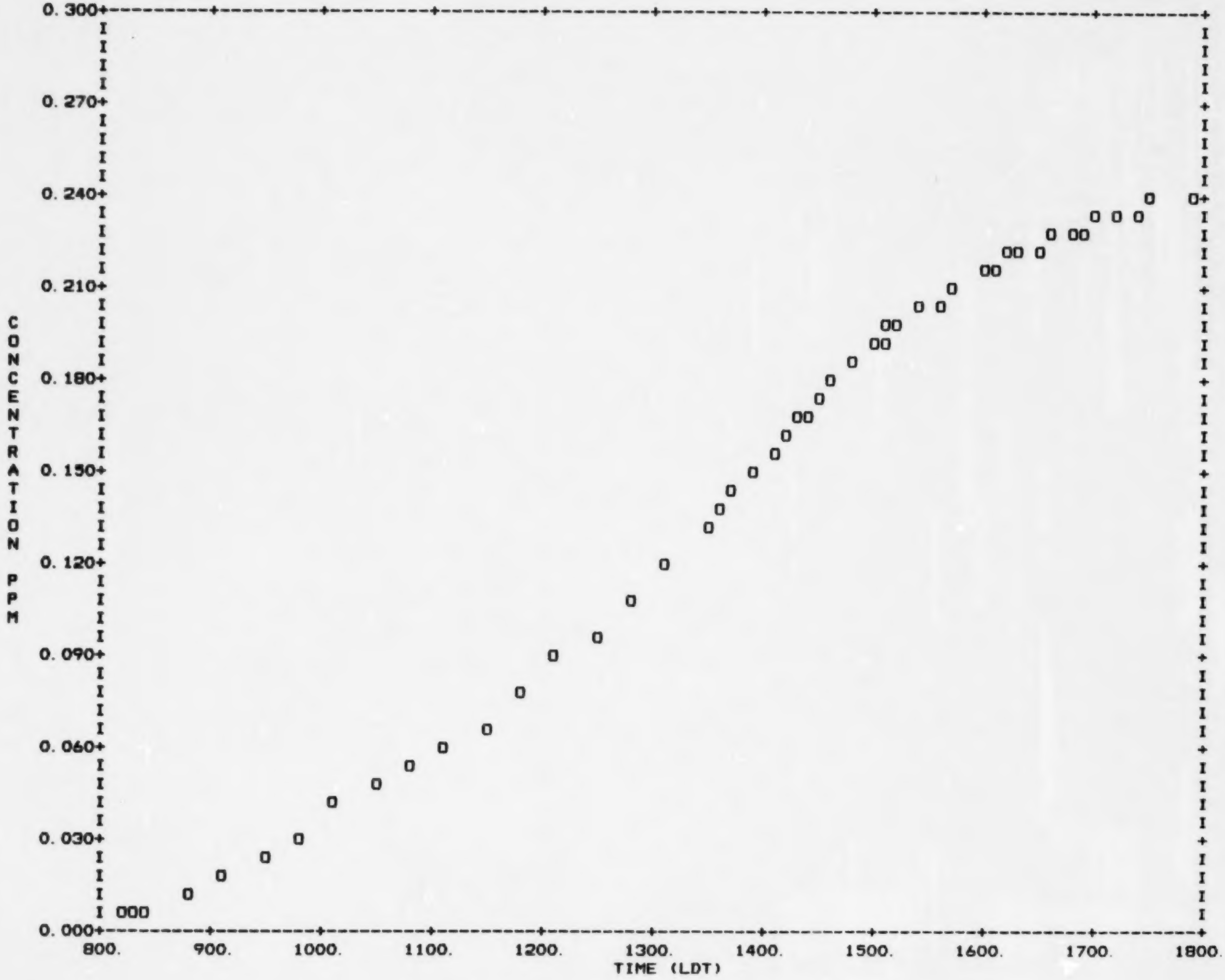
 THE PHOTOLYTIC RATE CONSTANTS ARE
          3. 726E-01   3. 701E-04   1. 565E-02   6. 706E-02   5. 216E-04   9. 687E 00   1. 714E 00   6. 173E-04   1. 130E-03
          1. 015E-04   1. 118E-01   1. 490E-05   1. 937E-03   5. 961E-04   2. 608E-04   7. 451E-03   1. 118E-04   1. 490E-03


 THE CURRENT MIXING HEIGHT IS     1235. 00

 THE CURRENT TEMPERATURE IS        303. 00

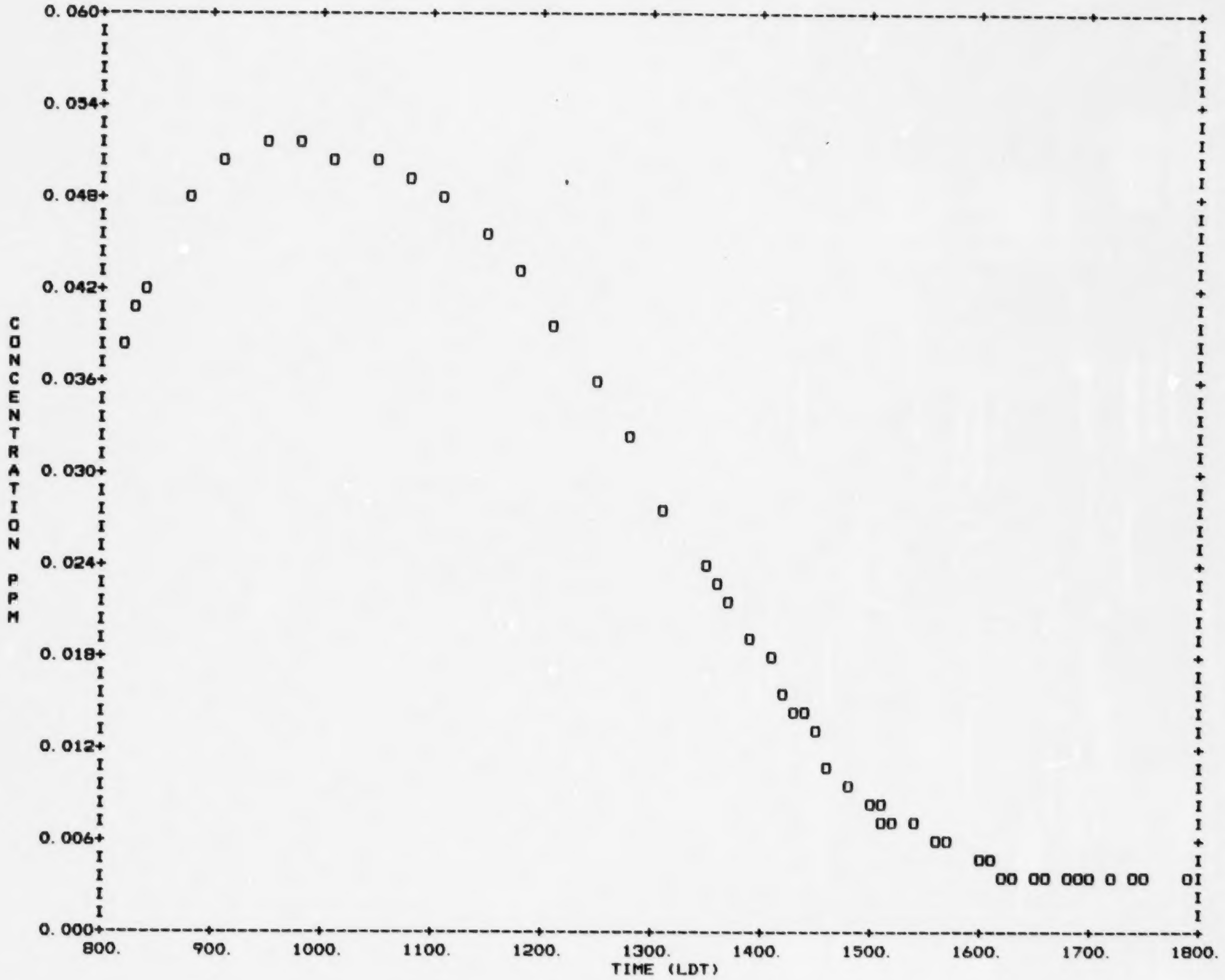
 THE CURRENT ZENITH ANGLE IS        63. 53
```

```
MAXIMUM O3     NOT REACHED, THE LAST ONE HOUR AVERAGE WAS 0. 23640 PPM.
MAXIMUM ONE HOUR AVE NO2    = 0. 05138 CENTERED AT  941.  LDT
MAXIMUM ONE HOUR AVE PAR    = 0. 49254 CENTERED AT  830.  LDT
```



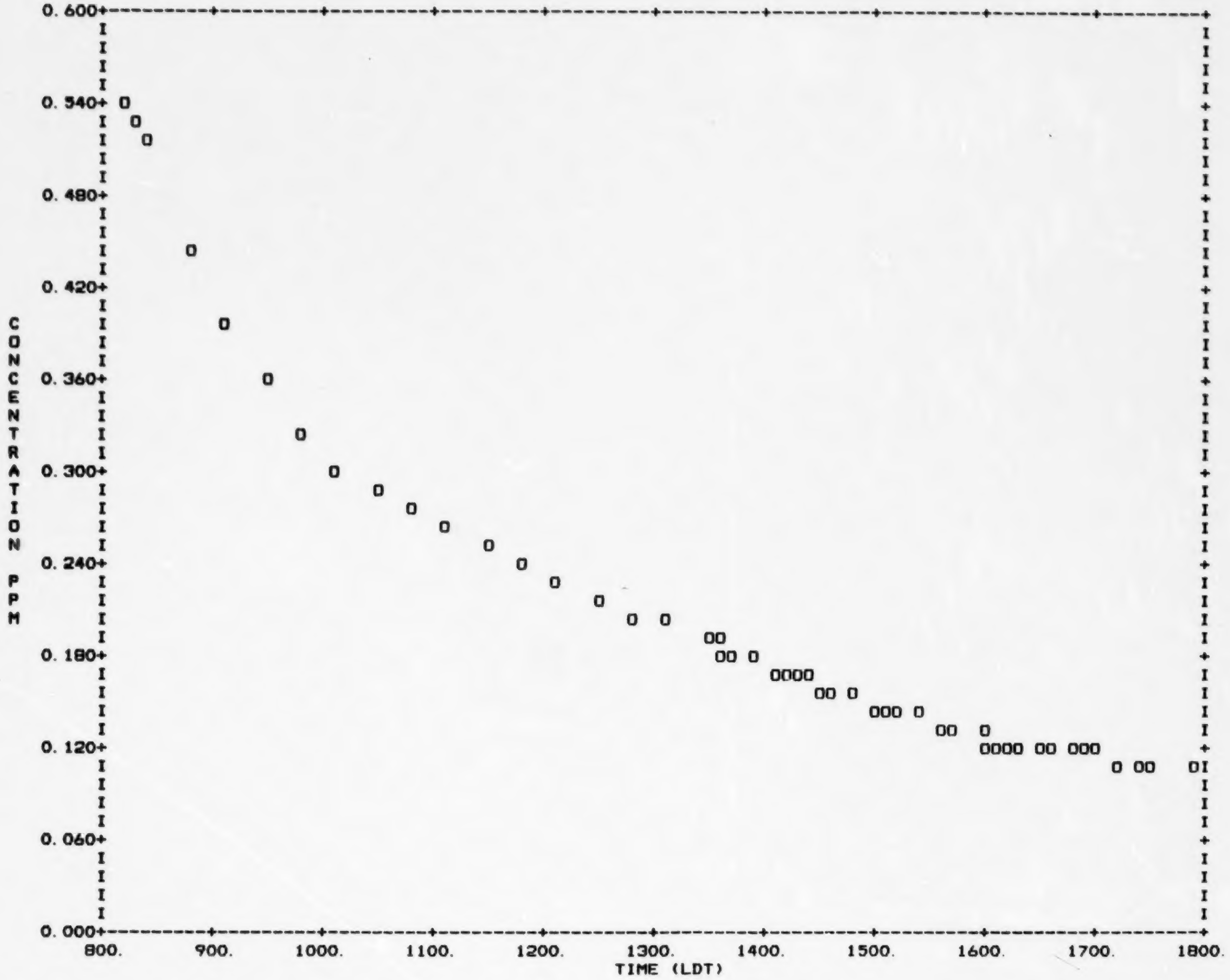
EXAMPLE 1 - TEST RUN USING EKMA/CBM-X

O3 CONCENTRATION AS A FUNCTION OF TIME



EXAMPLE 1 - TEST RUN USING EKMA/CBM-X

NO2 CONCENTRATION AS A FUNCTION OF TIME



EXAMPLE 1 - TEST RUN USING EKMA/CBM-X

PAR CONCENTRATION AS A FUNCTION OF TIME

EXAMPLE 2

CALC USING OPTIONAL MECHANISM

```

         1         2         3         4         5         6         7
123456789012345678901234567890123456789012345678901234567890123456789012

PLOT                          8.         5.6
MECH     82.        7.        7.        1.
1.        37.       38.       67.       76.       73.       71.
OLE       PAR       ARO       ETH       HCHO      DCRB      NR
2.        1.        6.        2.        1.        3.        1.
  1  NO2            NO   O               1.0
  2  O              O3                  4400000.
  3  NO   O3        NO2                 26.6      1450.
  4  NO2  O3        NO3                 .048      2450.
  5  NO2  O         NO                  13000.
  6  OH   O3        HO2                 100.      1000.
  7  HO2  O3        OH                  2.4       1525.
  8  OH   NO2       HNO3                 16000.
  9  OH   CO        HO2                  440.
 10  NO   NO        NO2  NO2            .00015
 11  NO   NO3       NO2  NO2            28000.
 12  NO2  NO3       HNO3 HNO3           26.0      -10600.
 13  NO   HO2       NO2  OH             12000.
 14  HO2  HO2       H2O2                15000.
 15  X    PAR                             100000.
 16  OH   PAR       MEO2                1200.      560.
 17  O    OLE       MEO2 ACO3 X         2700.      325.
 18  O    OLE       HCHO PAR            2700.      325.
 19  OH   OLE       RAO2                37000.    -540.
 20  O3   OLE       HCHO CRIG           .008      1900.
 21  O3   OLE       HCHO MCRG X         .008      1900.
 22  O    ETH       MEO2 HO2  CO        600.      800.
 23  O    ETH       HCHO PAR            600.      800.
 24  OH   ETH       RBO2                12000.    -382.
 25  O3   ETH       HCHO CRIG           .0024     2560.
 26  NO   ACO3      NO2  MEO2           10400.
 27  NO   RBO2      NO2  HCHO HO2  HCHO 12000.
 28  NO   RAO2      NO2  HCHO HO2  HCHO 12000.
 29  NO   MEO2      NO2  HCHO MEO2 X    3700.
 30  NO   MEO2      NO2  HCHO HO2       7400.
 31  NO   MEO2      NRAT                900.
 32  O3   RBO2      HCHO HCHO HO2       5.
 33  O3   RAO2      HCHO HCHO HO2       20.
 34  OH   HCHO      CRO2 X              100.
 35  OH   HCHO      HO2  CO             9000.
 36  OH   HCHO      ACO3 X              8200.
 37  HCHO           GG                  .564
 78  GG             HO2  HO2  CO        8867.
 79  GG             MEO2 MEO2 X    XCO  1133.
 38  HCHO           CO                  .24
 39  NO2  ACO3      PAN                 7000.
 40  PAN            ACO3 NO2            .022      13500.
 41  HO2  ACO3                          15000.
 42  HO2  MEO2                           9000.
 43  NO   CRIG      NO2  HCHO           12000.
 44  NO2  CRIG      NO3  HCHO           8000.
 45  HCHO CRIG                          2000.
 46  NO   MCRG      NO2  HCHO PAR       12000.
 47  NO2  MCRG      NO3  HCHO PAR       8000.
```

Exhibit 3

```
(        59)  48  HCHO MCRG                          2000.
(        60)  49  CRIG           CO                   670.
(        61)  50  CRIG                               240.
(        62)  51  CRIG           HO2  HO2  CO        90.
(        63)  52  MCRG                                150.
(        64)  53  MCRG           MEO2 OH   CO        340.
(        65)  54  MCRG           MEO2 HO2            425.
(        66)  55  MCRG           HCHO HO2  CO   HO2    85.
(        67)  56  OH   ARO       RARO                6000.       600.
(        68)  57  OH   ARO       HO2  OPEN           14500.      400.
(        69)  58  NO   RARO      NO2  PHEN HO2       4000.
(        70)  59  OPEN NO        NO2  DCRB X    APRC 6000.
(        71)  60  APRC           DCRB HCHO CO   X    10000.
(        72)  61  APRC           HCHO HCHO CO   CO   10000.
(        73)  62  PHEN NO3       PHO  HNO3           5000.0
(        74)  63  PHO  NO2       NPHN                4000.
(        75)  64  PHO  HO2       PHEN                50000.
(        76)  65  OPEN O3        DCRB X    APRC       40.0
(        77)  66  OH   PHEN      HO2  APRC PAR  HCHO 30000.
(        78)  67  DCRB           HO2  ACO3 CO        0.02
(        79)  68  PHEN OH        PHO                  10000.
(        80)  69  CRO2 NO        NO2  ACO3 HCHO X     12000.
(        81)  70  DCRB OH        ACO3 CO              25000.
(        82)  71  HONO           OH   NO              3.1
(        83)  72  OH   NO        HONO                9770.
(        84)  73  O3             O1D                  .54
(        85)  74  O1D            O                      4.44E10
(        86)  75  O1D            OH   OH                6.8E09
(        87)  76  O3             O                   1.0
(        88)  77  XCO            X    CO              10000.
(        89)  80  OH             HO2                     88.
(        90)  81  OH             MEO2                    28.
(        91)  82  NR             NR                       1.
(        92)  ZENITH        6.
(        93)  1.            0.85470   0.85470   0.84745   0.84033   0.82645   0.80000
(        94)     0.77520    0.71428   0.65359   0.62500
(        95)  38.           0.01091   0.01088   0.01074   0.01050   0.01014   0.00961
(        96)     0.00897    0.00785   0.00706   0.00694
(        97)  37.           0.00417   0.00415   0.00406   0.00390   0.00366   0.00334
(        98)     0.00290    0.00239   0.00198   0.00177
(        99)  76.           0.06449   0.06460   0.06478   0.06498   0.06580   0.06823
(       100)     0.07180    0.08285   0.09928   0.07422
(       101)  73.           0.00821   0.00807   0.00752   0.00666   0.00551   0.00415
(       102)     0.00268    0.00140   0.00065   0.00031
(       103)  71.           0.06333   0.06327   0.06310   0.06277   0.06225   0.06143
(       104)     0.06094    0.05810   0.05649   0.05852
(       105)  TITL
(       106)  EXAMPLE 2 - TEST RUN USING EKMA/CB-3
(       107)  PLACE      39.933     75.10      5.0        1980.      6.0        24.0
(       108)  TEST CITY
(       109)  DILU       250.       1235.                 1600.
(       110)  REAC       7.0
(       111)  0.03       0.58       0.19       0.04       0.050      0.000      0.150
(       112)  EMIS       -8.0       .17        .17        .17        .10        .02
(       113)  .02        .02        .02
(       114)  .35        .35        .35        .19        .03        .03        .03
(       115)  .07
(       116)  TRANS      .010       .070       -7.        -7.        0.0        0.0
(      117)  .038      .03      .53      .13      .05      .26      0.0
(      118)  0.0
(      119)  .040      .03      .61      .15      .06      .15      0.0
(      120)  0.0
(      121)  SPEC      3.
(      122)  03        NO2      PAR
(      123)  CALC      1.1      .12      1.
(      124)
(      125)      BLANK
```

```
****************************************
*                                      *
*   OZONE ISOPLETH PLOTTING PACKAGE    *
*       WITH OPTIONAL MECHANISMS       *
*                                      *
*              O Z I P M               *
*                                      *
*             VERSION 3.1              *
*                                      *
*           SEPTEMBER, 1985            *
*                                      *
****************************************
```

Exhibit 4

```
THE INPUTS FOR THIS RUN ARE

         PLOT                             8.         5. 6
         MECH        82.        7.        7.         1.
         1.         37.       38.        67.       76.        73.        71.
         OLE        PAR       ARO        ETH       HCHO       DCRB       NR
         2.         1.        6.         2.        1.         3.         1.
            1 NO2             NO    O                 1. 0
            2 O               O3                    4400000.
            3 NO    O3        NO2                   26. 6      1450.
            4 NO2   O3        NO3                   . 048      2450.
            5 NO2   O         NO                    13000.
            6 OH    O3        HO2                   100.       1000.
            7 HO2   O3        OH                    2. 4       1525.
            8 OH    NO2       HNO3                    16000.
            9 OH    CO        HO2                     440.
           10 NO    NO        NO2   NO2             . 00015
           11 NO    NO3       NO2   NO2             28000.
           12 NO2   NO3       HNO3  HNO3            26. 0      -10600.
           13 NO    HO2       NO2   OH              12000.
           14 HO2   HO2       H2O2                  15000.
           15 X     PAR                               100000.
           16 OH    PAR       MEO2                  1200.       560.
           17 O     OLE       MEO2  ACO3  X         2700.       325.
           18 O     OLE       HCHO  PAR             2700.       325.
           19 OH    OLE       RAO2                  37000.      -540.
           20 O3    OLE       HCHO  CRIG            . 008       1900.
           21 O3    OLE       HCHO  MCRG  X         . 008       1900.
           22 O     ETH       MEO2  HO2   CO        600.       800.
           23 O     ETH       HCHO  PAR             600.       800.
           24 OH    ETH       RBO2                  12000.     -382.
           25 O3    ETH       HCHO  CRIG            . 0024     2560.
           26 NO    ACO3      NO2   MEO2            10400.
           27 NO    RBO2      NO2   HCHO  HO2  HCHO 12000.
           28 NO    RAO2      NO2   HCHO  HO2  HCHO 12000.
           29 NO    MEO2      NO2   HCHO  MEO2 X    3700.
           30 NO    MEO2      NO2   HCHO  HO2       7400.
           31 NO    MEO2      NRAT                  900.
           32 O3    RBO2      HCHO  HCHO  HO2       5.
           33 O3    RAO2      HCHO  HCHO  HO2       20.
           34 OH    HCHO      CRO2  X               100.
           35 OH    HCHO      HO2   CO              9000.
           36 OH    HCHO      ACO3  X               8200.
           37 HCHO            GG                    . 564
           78 GG              HO2   HO2   CO        8867.
           79 GG              MEO2  MEO2  X    XCO  1133.
           38 HCHO            CO                    . 24
           39 NO2   ACO3      PAN                   7000.
           40 PAN             ACO3  NO2             . 022      13500.
           41 HO2   ACO3                            15000.
           42 HO2   MEO2                             9000.
```

```
THE INPUTS FOR THIS RUN ARE
         43  NO   CRIQ       NO2  HCHO            12000.
         44  NO2  CRIQ       NO3  HCHO            8000.
         45  HCHO CRIQ                            2000.
         46  NO   MCRQ       NO2  HCHO PAR        12000.
         47  NO2  MCRQ       NO3  HCHO PAR        8000.
         48  HCHO MCRQ                            2000.
         49  CRIQ            CO                    670.
         50  CRIQ                                 240.
         51  CRIQ            HO2  HO2  CO         90.
         52  MCRQ                                  150.
         53  MCRQ            MEO2 OH   CO         340.
         54  MCRQ            MEO2 HO2             425.
         55  MCRQ            HCHO HO2  CO   HO2     85.
         56  OH   ARO        RARO                 6000.       600.
         57  OH   ARO        HO2  OPEN            14500.      400.
         58  NO   RARO       NO2  PHEN HO2        4000.
         59  OPEN NO         NO2  DCRB X    APRC 6000.
         60  APRC            DCRB HCHO CO   X    10000.
         61  APRC            HCHO HCHO CO   CO   10000.
         62  PHEN NO3        PHO  HNO3            5000. 0
         63  PHO  NO2        NPHN                 4000.
         64  PHO  HO2        PHEN                 50000.
         65  OPEN O3         DCRB X    APRC        40. 0
         66  OH   PHEN       HO2  APRC PAR  HCHO 30000.
         67  DCRB            HO2  ACO3 CO        0. 02
         68  PHEN OH         PHO                   10000.
         69  CRO2 NO         NO2  ACO3 HCHO X      12000.
         70  DCRB OH         ACO3 CO               25000.
         71  HONO            OH   NO               3. 1
         72  OH   NO         HONO                  9770.
         73  O3              O1D                   . 54
         74  O1D             O                        4. 44E10
         75  O1D             OH   OH                  6. 8E09
         76  O3              O                     1. 0
         77  XCO             X    CO               10000.
         80  OH              HO2                      88.
         81  OH              MEO2                     28.
         82  NR              NR                        1.
        ZENITH          6.
        1.              0. 85470   0. 85470   0. 84745   0. 84033   0. 82645   0. 80000
           0. 77520     0. 71428   0. 65359   0. 62500
        38.             0. 01091   0. 01088   0. 01074   0. 01050   0. 01014   0. 00961
           0. 00897     0. 00785   0. 00706   0. 00694
        37.             0. 00417   0. 00415   0. 00406   0. 00390   0. 00366   0. 00334
           0. 00290     0. 00239   0. 00198   0. 00177
        76.             0. 06449   0. 06460   0. 06478   0. 06498   0. 06580   0. 06823
           0. 07180     0. 08285   0. 09928   0. 07422
        73.             0. 00821   0. 00807   0. 00752   0. 00666   0. 00551   0. 00415
           0. 00268     0. 00140   0. 00065   0. 00031
        71.             0. 06333   0. 06327   0. 06310   0. 06277   0. 06225   0. 06143
```

```
THE INPUTS FOR THIS RUN ARE

            0. 06094  0. 05810  0. 05649  0. 05852
         TITL
         EXAMPLE 2 - TEST RUN USING EKMA/CB-3
         PLACE     39. 933   75. 10    5. 0      1980.     6. 0      24. 0
         TEST CITY
         DILU      250.      1235.               1600.
         REAC      7. 0
         0. 03     0. 58     0. 19     0. 04     0. 050    0. 000    0. 150
         EMIS      -8. 0     . 17      . 17      . 17      . 10      . 02
         . 02      . 02      . 02
         . 35      . 35      . 35      . 19      . 03      . 03      . 03
         . 07
         TRANS     . 010     . 070     -7.       -7.       0. 0      0. 0
         . 038     . 03      . 53      . 13      . 05      . 26      0. 0
         0. 0
         . 040     . 03      . 61      . 15      . 06      . 15      0. 0
         0. 0
         SPEC      3.
         O3        NO2       PAR
         CALC      1. 1      . 12      1.
```

```
THE REACTIONS                                                                  RATE CONSTANT  ACT. ENERGY(K)
  1      NO2                     =     NO    +    O                            1.000E 00      0.000E-01
  2      O                       =     O3                                      4.400E 06      0.000E-01
  3      NO    +    O3           =     NO2                                     2.660E 01      1.450E 03
  4      NO2   +    O3           =     NO3                                     4.800E-02      2.450E 03
  5      NO2   +    O            =     NO                                      1.300E 04      0.000E-01
  6      OH    +    O3           =     HO2                                     1.000E 02      1.000E 03
  7      HO2   +    O3           =     OH                                      2.400E 00      1.525E 03
  8      OH    +    NO2          =     HNO3                                    1.600E 04      0.000E-01
  9      OH    +    CO           =     HO2                                     4.400E 02      0.000E-01
 10      NO    +    NO           =     NO2   +    NO2                          1.500E-04      0.000E-01
 11      NO    +    NO3          =     NO2   +    NO2                          2.800E 04      0.000E-01
 12      NO2   +    NO3          =     HNO3  +    HNO3                         2.600E 01     -1.060E 04
 13      NO    +    HO2          =     NO2   +    OH                           1.200E 04      0.000E-01
 14      HO2   +    HO2          =     H2O2                                    1.500E 04      0.000E-01
 15      X     +    PAR          =                                             1.000E 05      0.000E-01
 16      OH    +    PAR          =     MEO2                                    1.200E 03      5.600E 02
 17      O     +    OLE          =     MEO2  +    ACO3  +    X                 2.700E 03      3.250E 02
 18      O     +    OLE          =     HCHO  +    PAR                          2.700E 03      3.250E 02
 19      OH    +    OLE          =     RAO2                                    3.700E 04     -5.400E 02
 20      O3    +    OLE          =     HCHO  +    CRIG                         8.000E-03      1.900E 03
 21      O3    +    OLE          =     HCHO  +    MCRG  +    X                 8.000E-03      1.900E 03
 22      O     +    ETH          =     MEO2  +    HO2   +    CO                6.000E 02      8.000E 02
 23      O     +    ETH          =     HCHO  +    PAR                          6.000E 02      8.000E 02
 24      OH    +    ETH          =     RBO2                                    1.200E 04     -3.820E 02
 25      O3    +    ETH          =     HCHO  +    CRIG                         2.400E-03      2.560E 03
```

```
THE REACTIONS                                                                     RATE CONSTANT  ACT. ENERGY(K)
 26      NO    +    ACO3         =    NO2   +   MEO2                                1.040E 04      0.000E-01
 27      NO    +    RBO2         =    NO2   +   HCHO  +   HO2   +   HCHO            1.200E 04      0.000E-01
 28      NO    +    RAO2         =    NO2   +   HCHO  +   HO2   +   HCHO            1.200E 04      0.000E-01
 29      NO    +    MEO2         =    NO2   +   HCHO  +   MEO2  +   X               3.700E 03      0.000E-01
 30      NO    +    MEO2         =    NO2   +   HCHO  +   HO2                       7.400E 03      0.000E-01
 31      NO    +    MEO2         =    NRAT                                          9.000E 02      0.000E-01
 32      O3    +    RBO2         =    HCHO  +   HCHO  +   HO2                       5.000E 00      0.000E-01
 33      O3    +    RAO2         =    HCHO  +   HCHO  +   HO2                       2.000E 01      0.000E-01
 34      OH    +    HCHO         =    CRO2  +   X                                   1.000E 02      0.000E-01
 35      OH    +    HCHO         =    HO2   +   CO                                  9.000E 03      0.000E-01
 36      OH    +    HCHO         =    ACO3  +   X                                   8.200E 03      0.000E-01
 37      HCHO                    =    GG                                            5.640E-01      0.000E-01
 78      GG                      =    HO2   +   HO2   +   CO                        8.867E 03      0.000E-01
 79      GG                      =    MEO2  +   MEO2  +   X     +   XCO             1.133E 03      0.000E-01
 38      HCHO                    =    CO                                            2.400E-01      0.000E-01
 39      NO2   +    ACO3         =    PAN                                           7.000E 03      0.000E-01
 40      PAN                     =    ACO3  +   NO2                                 2.200E-02      1.350E 04
 41      HO2   +    ACO3         =                                                  1.500E 04      0.000E-01
 42      HO2   +    MEO2         =                                                  9.000E 03      0.000E-01
 43      NO    +    CRIG         =    NO2   +   HCHO                                1.200E 04      0.000E-01
 44      NO2   +    CRIG         =    NO3   +   HCHO                                8.000E 03      0.000E-01
 45      HCHO  +    CRIG         =                                                  2.000E 03      0.000E-01
 46      NO    +    MCRG         =    NO2   +   HCHO  +   PAR                       1.200E 04      0.000E-01
 47      NO2   +    MCRG         =    NO3   +   HCHO  +   PAR                       8.000E 03      0.000E-01
 48      HCHO  +    MCRG         =                                                  2.000E 03      0.000E-01
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THE REACTIONS                                                          RATE CONSTANT  ACT. ENERGY(K)
 49    CRIQ              =   CO                                         6.700E 02      0.000E-01
 50    CRIQ              =                                              2.400E 02      0.000E-01
 51    CRIQ              =   HO2   +  HO2   +  CO                       9.000E 01      0.000E-01
 52    MCRQ              =                                              1.500E 02      0.000E-01
 53    MCRQ              =   MEO2  +  OH    +  CO                       3.400E 02      0.000E-01
 54    MCRQ              =   MEO2  +  HO2                               4.250E 02      0.000E-01
 55    MCRQ              =   HCHO  +  HO2   +  CO    +  HO2             8.500E 01      0.000E-01
 56    OH    +  ARO      =   RARO                                       6.000E 03      6.000E 02
 57    OH    +  ARO      =   HO2   +  OPEN                              1.450E 04      4.000E 02
 58    NO    +  RARO     =   NO2   +  PHEN  +  HO2                      4.000E 03      0.000E-01
 59    OPEN  +  NO       =   NO2   +  DCRB  +  X     +  APRC            6.000E 03      0.000E-01
 60    APRC              =   DCRB  +  HCHO  +  CO    +  X               1.000E 04      0.000E-01
 61    APRC              =   HCHO  +  HCHO  +  CO    +  CO              1.000E 04      0.000E-01
 62    PHEN  +  NO3      =   PHO   +  HNO3                              5.000E 03      0.000E-01
 63    PHO   +  NO2      =   NPHN                                       4.000E 03      0.000E-01
 64    PHO   +  HO2      =   PHEN                                       5.000E 04      0.000E-01
 65    OPEN  +  O3       =   DCRB  +  X     +  APRC                     4.000E 01      0.000E-01
 66    OH    +  PHEN     =   HO2   +  APRC  +  PAR   +  HCHO            3.000E 04      0.000E-01
 67    DCRB              =   HO2   +  ACO3  +  CO                       2.000E-02      0.000E-01
 68    PHEN  +  OH       =   PHO                                        1.000E 04      0.000E-01
 69    CRO2  +  NO       =   NO2   +  ACO3  +  HCHO  +  X               1.200E 04      0.000E-01
 70    DCRB  +  OH       =   ACO3  +  CO                                2.500E 04      0.000E-01
 71    HONO              =   OH    +  NO                                3.100E 00      0.000E-01
 72    OH    +  NO       =   HONO                                       9.770E 03      0.000E-01
 73    O3                =   O1D                                        5.400E-01      0.000E-01
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THE REACTIONS                                                          RATE CONSTANT  ACT. ENERGY(K)
 74       O1D                =      O                                    4.440E 10      0.000E-01
 75       O1D                =      OH    +     OH                       6.800E 09      0.000E-01
 76       O3                 =      O                                    1.000E 00      0.000E-01
 77       XCO                =      X     +     CO                       1.000E 04      0.000E-01
 80       OH                 =      HO2                                  8.800E 01      0.000E-01
 81       OH                 =      MEO2                                 2.800E 01      0.000E-01
 82       NR                 =      NR                                   1.000E 00      0.000E-01
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                              THE FOLLOWING PHOTOLYSIS RATE CONSTANTS ARE USED

REACTION   SPECIES                                           ZENITH ANGLE (DEG)
   NO.                  0          10         20         30         40         50         60         70         78         86

    1        NO2     5. 13E-01  5. 09E-01  4. 96E-01  4. 74E-01  4. 39E-01  3. 88E-01  3. 17E-01  2. 06E-01  1. 01E-01  2. 18E-02
   37        HCHO    1. 21E-03  1. 19E-03  1. 14E-03  1. 04E-03  9. 07E-04  7. 31E-04  5. 18E-04  2. 77E-04  1. 13E-04  2. 18E-05
   38        HCHO    1. 34E-03  1. 33E-03  1. 28E-03  1. 19E-03  1. 07E-03  8. 95E-04  6. 82E-04  3. 88E-04  1. 72E-04  3. 63E-05
   67        DCRB    1. 03E-02  1. 02E-02  9. 93E-03  9. 48E-03  8. 79E-03  7. 76E-03  6. 34E-03  4. 12E-03  2. 03E-03  4. 36E-04
   76        O3      3. 31E-02  3. 29E-02  3. 21E-02  3. 08E-02  2. 89E-02  2. 65E-02  2. 27E-02  1. 71E-02  1. 01E-02  1. 62E-03
   73        O3      2. 27E-03  2. 22E-03  2. 02E-03  1. 71E-03  1. 31E-03  8. 70E-04  4. 59E-04  1. 56E-04  3. 56E-05  3. 65E-06
   71        HONO    1. 01E-01  9. 98E-02  9. 71E-02  9. 23E-02  8. 48E-02  7. 39E-02  5. 99E-02  3. 71E-02  1. 78E-02  3. 96E-03
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EXAMPLE 2 - TEST RUN USING EKMA/CB-3

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

        TEST CITY

LATITUDE      39.933

LONGITUDE     75.100

TIME ZONE     5.0

DATE          6      24     1980

TIME          800    TO     1800      LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS      INITIAL   250.      FINAL       1235.

TIMING                 START     800.      STOP        1600.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME       800      900      1000     1100     1200     1300     1400     1500     1600

HEIGHT     250.0    413.6    619.2    811.8    954.3    1055.0   1129.0   1186.6   1235.0


REACTIVITY

EMISSIONS        OLE   FRACTION 0.030    PAR  FRACTION 0.580    ARO  FRACTION 0.190

EMISSIONS        ETH   FRACTION 0.040    HCHO FRACTION 0.050    DCRB FRACTION 0.000

EMISSIONS        NR    FRACTION 0.150

SURFACE LAYER    OLE   FRACTION 0.030    PAR  FRACTION 0.530    ARO  FRACTION 0.130

SURFACE LAYER    ETH   FRACTION 0.050    HCHO FRACTION 0.260    DCRB FRACTION 0.000

SURFACE LAYER    NR    FRACTION 0.000

ALOFT            OLE   FRACTION 0.030    PAR  FRACTION 0.610    ARO  FRACTION 0.150

ALOFT            ETH   FRACTION 0.060    HCHO FRACTION 0.150    DCRB FRACTION 0.000

ALOFT            NR    FRACTION 0.000

NO2/NOX        0.250
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TRANSPORTED CONCENTRATIONS

SURFACE LAYER        OZONE   0.010     HYDROCARBON  0.038    NOX      0.000 PPM

ALOFT                OZONE   0.070     HYDROCARBON  0.040    NOX      0.000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES     HOUR          1     2     3     4     5     6     7     8

  VOC     FRACTION     0.170 0.170 0.170 0.100 0.020 0.020 0.020 0.020

  NOX     FRACTION     0.350 0.350 0.350 0.190 0.030 0.030 0.030 0.070
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                              EXAMPLE 2 - TEST RUN USING EKMA/CB-3
THE ERROR TOLERANCE IS  3.000E-03

THE TEMPERATURE USED IS  3.030E 02

THE MIXING HEIGHT IS  2.50E 02

THE RATE CONSTANTS USED WERE

    2.707E-01   4.400E 06   2.882E 01   5.497E-02   1.300E 04   1.057E 02   2.611E 00   1.600E 04   4.400E 02   1.500E-04
    2.800E 04   1.446E 01   1.200E 04   1.500E 04   1.000E 05   1.238E 03   2.749E 03   2.749E 03   3.591E 04   8.888E-03
    8.888E-03   6.272E 02   6.272E 02   1.175E 04   2.766E-03   1.040E 04   1.200E 04   1.200E 04   3.700E 03   7.400E 03
    9.000E 02   5.000E 00   2.000E 01   1.000E 02   9.000E 03   8.200E 03   4.081E-04   5.519E-04   7.000E 03   4.646E-02
    1.500E 04   9.000E 03   1.200E 04   8.000E 03   2.000E 03   1.200E 04   8.000E 03   2.000E 03   6.700E 02   2.400E 02
    9.000E 01   1.500E 02   3.400E 02   4.250E 02   8.500E 01   6.203E 03   1.482E 04   4.000E 03   6.000E 03   1.000E 04
    1.000E 04   5.000E 03   4.000E 03   5.000E 04   4.000E 01   3.000E 04   5.413E-03   1.000E 04   1.200E 04   2.500E 04
    5.022E-02   9.770E 03   3.002E-04   4.440E 10   6.800E 09   2.015E-02   1.000E 04   8.867E 03   1.133E 03   8.800E 01
    2.800E 01   1.000E 00
THE PHOTOLYSIS REACTIONS ARE

           1          37          38          67          76          73          71

THE PHOTOLYTIC RATE CONSTANTS ARE
        2.707E-01   4.081E-04   5.519E-04   5.413E-03   2.015E-02   3.002E-04   5.022E-02
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       TIME      NMOC       NMOC/       NOX        NO2         O3         NO2         PAR
      (LDT )     TOTAL       NOX       TOTAL     FRACTION   (INSTANT)  (INSTANT)   (INSTANT)

       800.     1.18200     9.85000     0.12000    0.25000    0.01000     0.03000     0.65814

   TIME          NO2         NO          O           O3          NO3         OH          HO2         HNO3        CO          H2O2
 INTERVAL        X           PAR         MEO2        OLE         ACO3        HCHO        RAO2        CRIG        MCRG        ETH
                 RBO2        NRAT        CRO2        GQ        , PAN         ARO         RARO        OPEN        PHEN        DCRB
                 APRC        PHO         NPHN        HONO        O1D         XCO         NR

  8.000E 02   3.000E-02   9.000E-02   0.000E-01   1.000E-02   0.000E-01   0.000E-01   0.000E-01   0.000E-01   0.000E-01   0.000E-01
  1.000E-10   0.000E-01   6.581E-01   0.000E-01   1.707E-02   0.000E-01   6.488E-02   0.000E-01   0.000E-01   0.000E-01   2.295E-02
              0.000E-01   0.000E-01   0.000E-01   0.000E-01   0.000E-01   3.566E-02   0.000E-01   0.000E-01   0.000E-01   0.000E-01
              0.000E-01   0.000E-01   0.000E-01   0.000E-01   0.000E-01   0.000E-01   1.650E-01

 NET RATES    1.759E-02  -1.791E-02   8.321E-03  -2.567E-02   1.649E-05   0.000E-01   0.000E-01   0.000E-01   3.581E-05   0.000E-01
              1.517E-06  -3.450E-03   0.000E-01  -9.293E-05   0.000E-01  -3.913E-04   0.000E-01   2.152E-06   1.517E-06  -1.188E-04
              0.000E-01   0.000E-01   0.000E-01   2.648E-05   0.000E-01  -1.888E-04   0.000E-01   0.000E-01   0.000E-01   0.000E-01
              0.000E-01   0.000E-01   0.000E-01   0.000E-01   3.002E-06   0.000E-01  -9.015E-04

 THE REACTION RATES ARE
        8.12E-03    0.00E-01    2.59E-02    1.65E-05    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    1.21E-06
        0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    1.52E-06
        1.52E-06    0.00E-01    0.00E-01    0.00E-01    6.35E-07    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
        0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    2.65E-05    3.58E-05    0.00E-01    0.00E-01
        0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
        0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
        0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
        0.00E-01    0.00E-01    3.00E-06    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01    0.00E-01
        0.00E-01    1.65E-01                0.00E-01    0.00E-01    2.02E-04    0.00E-01    0.00E-01    0.00E-01    0.00E-01

 THE PHOTOLYTIC RATE CONSTANTS ARE
           2.707E-01   4.081E-04   5.519E-04   5.413E-03   2.015E-02   3.002E-04   5.022E-02


 THE CURRENT MIXING HEIGHT IS      250.00

 THE CURRENT TEMPERATURE IS        303.00

 THE CURRENT ZENITH ANGLE IS        64.62
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      TIME      NMOC       NMOC/        NOX         NO2          O3          NO2          PAR
     (LDT )     TOTAL       NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

     900.      0. 83756    8. 83779    0. 09477    0. 57634    0. 01753    0. 05462    0. 46711

   TIME        NO2         NO          O           O3          NO3         OH          HO2         HNO3        CO          H2O2
 INTERVAL      X           PAR         MEO2        OLE         ACO3        HCHO        RAO2        CRIG        MCRG        ETH
               RBO2        NRAT        CRO2        GQ          PAN         ARO         RARO        OPEN        PHEN        DCRB
               APRC        PHO         NPHN        HONO        O1D         XCO         NR

  9. 000E 02   5. 462E-02  4. 015E-02  4. 676E-09  1. 753E-02  4. 714E-08  8. 359E-08  6. 210E-07  2. 340E-03  7. 198E-03  1. 258E-07
  1. 571E 01   2. 875E-09  4. 671E-01  2. 899E-07  1. 077E-02  8. 851E-08  5. 231E-02  6. 738E-08  1. 211E-09  8. 282E-10  1. 598E-02
               3. 272E-08  4. 072E-04  9. 116E-10  3. 491E-09  4. 251E-04  2. 384E-02  7. 734E-08  1. 229E-07  4. 811E-04  1. 523E-03
               1. 540E-09  2. 355E-09  1. 096E-05  4. 800E-04  2. 514E-16  3. 955E-10  1. 170E-01

 NET RATES     2. 804E-04 -6. 950E-04  3. 548E-06  1. 770E-04  3. 875E-07  1. 912E-06 -6. 560E-07  5. 497E-05  1. 234E-04  4. 802E-09
               3. 314E-07 -2. 544E-03 -2. 666E-07 -8. 706E-05 -2. 126E-07 -1. 420E-04 -1. 700E-07  1. 824E-09  1. 730E-09 -9. 426E-05
              -7. 688E-08  7. 298E-06 -1. 947E-09 -4. 600E-09  1. 077E-05 -1. 606E-04 -6. 079E-08 -1. 485E-07  6. 944E-06  1. 880E-05
               9. 822E-08  1. 006E-09  4. 289E-07 -4. 594E-06 -3. 619E-08  9. 095E-13 -6. 311E-04


 THE REACTION RATES ARE
       2. 01E-02    2. 06E-02    2. 03E-02    5. 26E-05    3. 32E-06    1. 55E-07    2. 84E-08    7. 31E-05    2. 65E-07    2. 42E-07
       5. 30E-05    3. 72E-08    2. 99E-04    5. 78E-09    1. 34E-04    4. 83E-05    1. 38E-07    1. 38E-07    3. 23E-05    1. 68E-06
       1. 68E-06    4. 69E-08    4. 69E-08    1. 57E-05    7. 75E-07    3. 70E-05    1. 58E-05    3. 25E-05    4. 31E-05    8. 61E-05
       1. 05E-05    2. 87E-09    2. 36E-08    4. 37E-07    3. 94E-05    3. 59E-05    3. 49E-05    4. 36E-05    3. 38E-05    1. 97E-05
       8. 24E-10    1. 62E-09    5. 83E-07    5. 29E-07    1. 27E-07    3. 99E-07    3. 62E-07    8. 67E-08    8. 11E-07    2. 91E-07
       1. 09E-07    1. 24E-07    2. 82E-07    3. 52E-07    7. 04E-08    1. 24E-05    2. 95E-05    1. 24E-05    2. 96E-05    1. 54E-05
       1. 54E-05    1. 13E-07    5. 14E-07    7. 31E-11    8. 62E-08    1. 21E-06    1. 12E-05    4. 02E-07    4. 39E-07    3. 18E-06
       3. 36E-05    3. 28E-05    1. 28E-05    1. 12E-05    1. 71E-06    4. 47E-04    3. 95E-06    3. 10E-05    3. 95E-06    7. 36E-06
       2. 34E-06    1. 17E-01

 THE PHOTOLYTIC RATE CONSTANTS ARE
         3. 684E-01     6. 672E-04     8. 344E-04     7. 368E-03     2. 552E-02     7. 321E-04     7. 008E-02


 THE CURRENT MIXING HEIGHT IS      413. 60

 THE CURRENT TEMPERATURE IS        303. 00

 THE CURRENT ZENITH ANGLE IS        53. 19
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     TIME       NMOC        NMOC/        NOX          NO2         O3          NO2         PAR
    (LDT )     TOTAL         NOX        TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

    1000.     0.63213     8.50624     0.07431     0.73678     0.04068     0.05475     0.35353

  TIME          NO2          NO           O            O3           NO3          OH           HO2          HNO3         CO           H2O2
INTERVAL        X            PAR          MEO2         OLE          ACO3         HCHO         RAO2         CRIQ         MCRQ         ETH
                RBO2         NRAT         CRO2         QQ           PAN          ARO          RARO         OPEN         PHEN         DCRB
                APRC         PHO          NPHN         HONO         O1D          XCO          NR

 1.000E 03   5.475E-02    1.956E-02    5.645E-09    4.068E-02    2.181E-07    1.150E-07    1.397E-06    5.994E-03    1.464E-02    8.960E-07
 2.000E 01   4.215E-09    3.535E-01    6.566E-07    6.766E-03    2.175E-07    4.649E-02    1.170E-07    2.140E-09    1.392E-09    1.170E-02
             6.567E-08    8.327E-04    2.196E-09    4.092E-09    1.258E-03    1.655E-02    1.477E-07    2.324E-07    7.732E-04    2.211E-03
             1.550E-09    7.875E-09    6.226E-05    2.838E-04    9.770E-16    4.637E-10    8.926E-02

NET RATES   -4.188E-04    1.429E-04    2.222E-06    7.284E-04    3.529E-06   -8.499E-06    4.793E-06    6.835E-05    1.289E-04    2.424E-08
            -1.634E-06   -1.311E-03    1.681E-06   -4.873E-05    7.100E-07   -5.917E-05    3.904E-07   -1.654E-08   -1.265E-08   -5.091E-05
             3.845E-07    6.891E-06    1.919E-08   -3.538E-08    1.790E-05   -8.730E-05    2.489E-07    5.579E-07    2.820E-06    5.309E-06
            -6.833E-07    7.065E-09    1.376E-06   -3.203E-06    1.238E-07    9.095E-13   -3.115E-04


THE REACTION RATES ARE
        2.36E-02     2.48E-02     2.29E-02     1.22E-04     4.02E-06     4.94E-07     1.48E-07     1.01E-04     7.41E-07     5.74E-08
        1.19E-04     1.73E-07     3.28E-04     2.93E-08     1.49E-04     5.03E-05     1.05E-07     1.05E-07     2.79E-05     2.45E-06
        2.45E-06     4.14E-08     4.14E-08     1.58E-05     1.32E-06     4.43E-05     1.54E-05     2.75E-05     4.75E-05     9.50E-05
        1.16E-05     1.34E-08     9.52E-08     5.35E-07     4.81E-05     4.38E-05     4.09E-05     4.85E-05     8.34E-05     5.84E-05
        4.56E-09     8.25E-09     5.02E-07     9.37E-07     1.99E-07     3.27E-07     6.10E-07     1.29E-07     1.43E-06     5.14E-07
        1.93E-07     2.09E-07     4.73E-07     5.92E-07     1.18E-07     1.18E-05     2.82E-05     1.16E-05     2.73E-05     1.55E-05
        1.55E-05     8.43E-07     1.72E-06     5.50E-10     3.78E-07     2.67E-06     1.91E-05     8.89E-07     5.16E-07     6.36E-06
        2.36E-05     2.20E-05     5.01E-05     4.34E-05     6.64E-06     1.16E-03     4.64E-06     3.63E-05     4.64E-06     1.01E-05
        3.22E-06     8.93E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
           4.318E-01     8.795E-04     1.042E-03     8.635E-03     2.854E-02     1.233E-03     8.312E-02


THE CURRENT MIXING HEIGHT IS       619.16

THE CURRENT TEMPERATURE IS         303.00

THE CURRENT ZENITH ANGLE IS         41.73
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     TIME      NMOC        NMOC/        NOX         NO2          O3          NO2         PAR
     (LDT )    TOTAL        NOX        TOTAL      FRACTION    (INSTANT)   (INSTANT)   (INSTANT)

     1100.    0.52914     8.72761     0.06063     0.80762     0.06683     0.04896     0.29712

  TIME           NO2          NO           O            O3           NO3          OH           HO2          HNO3         CO           H2O2
INTERVAL         X            PAR          MEO2         OLE          ACO3         HCHO         RAO2         CRIG         MCRG         ETH
                 RBO2         NRAT         CRO2         GG           PAN          ARO          RARO         OPEN         PHEN         DCRB
                 APRC         PHO          NPHN         HONO         O1D          XCO          NR

 1.100E 03   4.896E-02    1.166E-02    5.741E-09    6.683E-02    5.482E-07    1.555E-07    2.781E-06    1.071E-02    2.351E-02    4.580E-06
 2.000E 01   5.897E-09    2.971E-01    1.333E-06    4.474E-03    4.576E-07    4.523E-02    1.768E-07    2.705E-09    1.636E-09    9.381E-03
             1.223E-07    1.330E-03    5.033E-09    4.680E-09    2.601E-03    1.250E-02    2.586E-07    3.969E-07    8.858E-04    2.476E-03
             1.647E-09    1.941E-08    2.007E-04    1.924E-04    2.193E-15    5.302E-10    7.662E-02

NET RATES   -1.018E-04   -1.278E-04    3.869E-06    4.500E-04   -2.806E-07    4.640E-07   -2.775E-07    8.798E-05    1.661E-04    1.002E-07
             5.838E-08   -7.443E-04   -6.666E-08   -3.281E-05   -6.586E-08   -9.221E-07    3.839E-09    3.363E-09    2.677E-09   -3.254E-05
            -1.322E-08    9.388E-06   -9.580E-10    8.956E-09    2.700E-05   -5.740E-05   -4.920E-09   -1.100E-08    1.063E-06    3.735E-06
             3.037E-08    1.135E-09    3.107E-06   -6.093E-07   -2.892E-08    1.819E-12   -1.548E-04


THE REACTION RATES ARE
        2.31E-02      2.53E-02      2.25E-02      1.80E-04      3.65E-06      1.10E-06      4.85E-07      1.22E-04      1.61E-06      2.04E-08
        1.79E-04      3.88E-07      3.89E-04      1.16E-07      1.75E-04      5.72E-05      7.06E-08      7.06E-08      2.50E-05      2.66E-06
        2.66E-06      3.38E-08      3.38E-08      1.71E-05      1.73E-06      5.55E-05      1.71E-05      2.47E-05      5.75E-05      1.15E-04
        1.40E-05      4.09E-08      2.36E-07      7.03E-07      6.33E-05      5.77E-05      4.68E-05      5.37E-05      1.57E-04      1.21E-04
        1.91E-08      3.34E-08      3.79E-07      1.06E-06      2.45E-07      2.29E-07      6.41E-07      1.48E-07      1.81E-06      6.49E-07
        2.43E-07      2.45E-07      5.56E-07      6.96E-07      1.39E-07      1.21E-05      2.88E-05      1.21E-05      2.78E-05      1.65E-05
        1.65E-05      2.43E-06      3.80E-06      2.70E-09      1.06E-06      4.13E-06      2.34E-05      1.38E-06      7.04E-07      9.63E-06
        1.77E-05      1.77E-05      1.12E-04      9.74E-05      1.49E-05      2.05E-03      5.30E-06      4.15E-05      5.30E-06      1.37E-05
        4.35E-06      7.66E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
          4.721E-01     1.035E-03     1.188E-03     9.443E-03     3.069E-02     1.680E-03     9.184E-02


THE CURRENT MIXING HEIGHT IS       811.78

THE CURRENT TEMPERATURE IS         303.00

THE CURRENT ZENITH ANGLE IS         30.69
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          TIME      NMOC       NMOC/        NOX         NO2         O3          NO2         PAR
         (LDT )     TOTAL      NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

         1200.     0.45977   10.04408     0.04577     0.86093     0.10023     0.03941     0.25935

  TIME           NO2         NO          O           O3          NO3         OH          HO2         HNO3        CO          H2O2
INTERVAL         X           PAR         MEO2        OLE         ACO3        HCHO        RAO2        CRIG        MCRG        ETH
                 RBO2        NRAT        CRO2        GG          PAN         ARO         RARO        OPEN        PHEN        DCRB
                 APRC        PHO         NPHN        HONO        O1D         XCO         NR

 1.200E 03   3.941E-02   6.366E-03   5.197E-09   1.002E-01   1.167E-06   2.165E-07   5.770E-06   1.686E-02   3.555E-02   2.136E-05
 2.000E 01   8.303E-09   2.593E-01   2.843E-06   2.759E-03   9.904E-07   4.584E-02   2.717E-07   3.095E-09   1.670E-09   7.603E-03
             2.428E-07   2.027E-03   1.225E-08   5.167E-09   4.857E-03   9.364E-03   4.801E-07   7.005E-07   8.506E-04   2.647E-03
             1.790E-09   4.263E-08   4.916E-04   1.462E-04   3.874E-15   5.855E-10   6.973E-02

NET RATES   -3.707E-04   9.704E-05  -1.301E-05   7.699E-04   5.052E-06  -1.744E-05   1.155E-05   1.078E-04   2.193E-04   4.551E-07
            -3.376E-06  -6.424E-04   3.848E-06  -2.771E-05   9.626E-06  -4.102E-06   1.466E-07  -2.607E-08  -1.986E-08  -3.051E-05
             6.755E-07   1.207E-05   5.697E-08  -2.992E-09   3.748E-05  -5.322E-05   3.489E-07   4.900E-07  -1.860E-06   1.476E-06
            -7.116E-07   7.145E-08   5.699E-06  -9.615E-07   3.989E-07   9.095E-13  -1.127E-04


THE REACTION RATES ARE
     1.95E-02     2.29E-02     1.84E-02     2.17E-04     2.66E-06     2.29E-06     1.51E-06     1.37E-04     3.39E-06     6.08E-09
     2.08E-04     6.65E-07     4.41E-04     4.99E-07     2.15E-04     6.95E-05     3.94E-08     3.94E-08     2.14E-05     2.46E-06
     2.46E-06     2.48E-08     2.48E-08     1.93E-05     2.11E-06     6.56E-05     1.85E-05     2.08E-05     6.70E-05     1.34E-04
     1.63E-05     1.22E-07     5.45E-07     9.93E-07     8.93E-05     8.14E-05     5.17E-05     5.83E-05     2.73E-04     2.26E-04
     8.57E-08     1.48E-07     2.36E-07     9.76E-07     2.84E-07     1.28E-07     5.27E-07     1.53E-07     2.07E-06     7.43E-07
     2.79E-07     2.51E-07     5.68E-07     7.10E-07     1.42E-07     1.26E-05     3.01E-05     1.22E-05     2.68E-05     1.79E-05
     1.79E-05     4.96E-06     6.72E-06     1.23E-08     2.81E-06     5.53E-06     2.62E-05     1.84E-06     9.36E-07     1.43E-05
     1.41E-05     1.35E-05     1.99E-04     1.72E-04     2.63E-05     3.21E-03     5.85E-06     4.58E-05     5.85E-06     1.91E-05
     6.06E-06     6.97E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
        4.941E-01     1.127E-03     1.271E-03     9.883E-03     3.202E-02     1.983E-03     9.661E-02


THE CURRENT MIXING HEIGHT IS      954.30

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        21.20
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          TIME        NMOC        NMOC/        NOX          NO2           O3            NO2           PAR
         (LDT )       TOTAL        NOX         TOTAL      FRACTION     (INSTANT)     (INSTANT)     (INSTANT)

         1300.       0. 39276    13. 68855    0. 02869    0. 89306      0. 14314      0. 02562      0. 22265

    TIME          NO2          NO           O            O3           NO3          OH           HO2          HNO3         CO           H2O2
 INTERVAL         X            PAR          MEO2         OLE          ACO3         HCHO         RAO2         CRIG         MCRG         ETH
                  RBO2         NRAT         CRO2         GG           PAN          ARO          RARO         OPEN         PHEN         DCRB
                  APRC         PHO          NPHN         HONO         O1D          XCO          NR

 1. 300E 03    2. 562E-02   3. 068E-03   4. 038E-09   1. 431E-01   2. 321E-06   3. 153E-07   1. 351E-05   2. 352E-02   5. 075E-02   1. 067E-04
 2. 000E 01    1. 209E-08   2. 226E-01   6. 936E-06   1. 395E-03   2. 449E-06   4. 566E-02   4. 190E-07   3. 031E-09   1. 303E-09   5. 808E-03
               5. 416E-07   2. 962E-03   3. 425E-08   5. 298E-09   8. 438E-03   6. 341E-03   9. 808E-07   1. 269E-06   6. 412E-04   2. 598E-03
               1. 780E-09   9. 111E-08   9. 504E-04   9. 688E-05   5. 864E-15   6. 003E-10   6. 421E-02
NET RATES      6. 647E-04  -8. 979E-04  -6. 764E-06  -1. 654E-04  -5. 236E-06  -3. 886E-05   2. 340E-05   1. 069E-04   2. 696E-04   2. 593E-06
              -7. 361E-06  -5. 652E-04   9. 401E-06  -1. 913E-05   3. 995E-05  -3. 277E-05  -8. 377E-07   3. 350E-08   3. 774E-08  -2. 829E-05
               1. 185E-06   1. 518E-05   1. 787E-07  -2. 301E-08   3. 594E-05  -4. 645E-05   3. 610E-07  -9. 990E-07  -4. 289E-06  -1. 597E-06
               1. 106E-06   6. 337E-08   8. 064E-06  -1. 964E-07   4. 098E-07   9. 095E-13  -7. 313E-05

THE REACTION RATES ARE
       1. 29E-02    1. 78E-02    1. 27E-02    2. 02E-04    1. 35E-06    4. 77E-06    5. 05E-06    1. 29E-04    7. 04E-06    1. 41E-09
       1. 99E-04    8. 60E-07    4. 97E-04    2. 74E-06    2. 69E-04    8. 69E-05    1. 55E-08    1. 55E-08    1. 58E-05    1. 77E-06
       1. 77E-06    1. 47E-08    1. 47E-08    2. 15E-05    2. 30E-06    7. 82E-05    1. 99E-05    1. 54E-05    7. 87E-05    1. 57E-04
       1. 92E-05    3. 88E-07    1. 20E-06    1. 44E-06    1. 30E-04    1. 18E-04    5. 30E-05    5. 94E-05    4. 39E-04    3. 92E-04
       4. 96E-07    8. 43E-07    1. 12E-07    6. 21E-07    2. 77E-07    4. 80E-08    2. 67E-07    1. 19E-07    2. 03E-06    7. 27E-07
       2. 73E-07    1. 95E-07    4. 43E-07    5. 54E-07    1. 11E-07    1. 24E-05    2. 96E-05    1. 20E-05    2. 34E-05    1. 78E-05
       1. 78E-05    7. 44E-06    9. 34E-06    6. 15E-08    7. 27E-06    6. 06E-06    2. 61E-05    2. 02E-06    1. 26E-06    2. 05E-05
       9. 52E-06    9. 45E-06    3. 01E-04    2. 60E-04    3. 99E-05    4. 65E-03    6. 00E-06    4. 70E-05    6. 00E-06    2. 77E-05
       8. 83E-06    6. 42E-02
THE PHOTOLYTIC RATE CONSTANTS ARE
          5. 016E-01    1. 160E-03    1. 300E-03    1. 003E-02    3. 246E-02    2. 100E-03    9. 825E-02


THE CURRENT MIXING HEIGHT IS      1055. 00

THE CURRENT TEMPERATURE IS         303. 00

THE CURRENT ZENITH ANGLE IS         16. 54
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       TIME      NMOC       NMOC/        NOX         NO2          O3          NO2          PAR
      (LDT )     TOTAL       NOX        TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

      1400.     0.33699    23.50250    0.01434     0.92600     0.18528     0.01328     0.19207


   TIME          NO2         NO          O           O3          NO3         OH          HO2         HNO3        CO          H2O2
 INTERVAL        X           PAR         MEO2        OLE         ACO3        HCHO        RAO2        CRIG        MCRG        ETH
                 RBO2        NRAT        CRO2        GG          PAN         ARO         RARO        OPEN        PHEN        DCRB
                 APRC        PHO         NPHN        HONO        O1D         XCO         NR

 1.400E 03   1.328E-02   1.061E-03   2.920E-09   1.853E-01   4.249E-06   3.586E-07   3.568E-05   2.857E-02   6.703E-02   7.085E-04
 1.000E 01   1.343E-08   1.921E-01   2.063E-05   6.114E-04   7.414E-06   4.344E-02   4.841E-07   2.658E-09   8.321E-10   4.300E-03
             1.325E-06   4.007E-03   1.215E-07   4.920E-09   1.294E-02   4.034E-03   2.113E-06   1.563E-06   3.713E-04   2.201E-03
             1.269E-09   1.680E-07   1.445E-03   4.592E-05   7.245E-15   5.574E-10   6.086E-02

NET RATES   -1.585E-04  -4.408E-05  -2.421E-08   5.734E-04   6.493E-07  -5.591E-07   1.217E-06   5.847E-05   2.524E-04   1.842E-05
             2.064E-07  -4.519E-04   6.022E-07  -8.690E-06  -2.906E-06  -6.265E-05  -8.472E-08   4.810E-09   3.394E-09  -2.167E-05
             1.863E-08   1.588E-05   1.024E-08   7.533E-09   7.562E-05  -3.074E-05   5.077E-09  -9.091E-08  -4.302E-06  -9.408E-06
             1.456E-07  -1.563E-09   7.544E-06  -7.755E-07   1.776E-07   0.000E-01  -4.584E-05


THE REACTION RATES ARE
      6.58E-03     1.28E-02     5.67E-03     1.35E-04     5.04E-07     7.02E-06     1.73E-05     7.62E-05     1.06E-05     1.69E-10
      1.26E-04     8.16E-07     4.54E-04     1.91E-05     2.58E-04     8.53E-05     4.91E-09     4.91E-09     7.87E-06     1.01E-06
      1.01E-06     7.87E-09     7.87E-09     1.81E-05     2.20E-06     8.18E-05     1.69E-05     6.16E-06     8.10E-05     1.62E-04
      1.97E-05     1.23E-06     1.79E-06     1.56E-06     1.40E-04     1.28E-04     4.92E-05     5.54E-05     6.89E-04     6.01E-04
      3.97E-06     6.62E-06     3.38E-08     2.82E-07     2.31E-07     1.06E-08     8.84E-08     7.23E-08     1.78E-06     6.38E-07
      2.39E-07     1.25E-07     2.83E-07     3.54E-07     7.07E-08     8.97E-06     2.14E-05     8.97E-06     9.95E-06     1.27E-05
      1.27E-05     7.89E-06     8.92E-06     3.00E-07     1.16E-05     3.99E-06     2.18E-05     1.33E-06     1.55E-06     1.97E-05
      4.45E-06     3.72E-06     3.71E-04     3.22E-04     4.93E-05     5.95E-03     5.57E-06     4.36E-05     5.57E-06     3.16E-05
      1.00E-05     6.09E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
        4.955E-01    1.133E-03    1.276E-03    9.909E-03    3.210E-02    2.003E-03    9.690E-02


THE CURRENT MIXING HEIGHT IS     1128.96

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        20.46
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            TIME     NMOC       NMOC/        NOX         NO2          O3          NO2          PAR
            (LDT )   TOTAL      NOX          TOTAL       FRACTION     (INSTANT)   (INSTANT)    (INSTANT)

            1500.    0.29676    44.22813     0.00671     0.94016      0.21052     0.00631      0.17031

  TIME          NO2          NO           O            O3           NO3          OH           HO2          HNO3         CO           H2O2
INTERVAL        X            PAR          MEO2         OLE          ACO3         HCHO         RAO2         CRIQ         MCRG         ETH
                RBO2         NRAT         CRO2         GG           PAN          ARO          RARO         OPEN         PHEN         DCRB
                APRC         PHO          NPHN         HONO         O1D          XCO          NR

 1.500E 03    6.308E-03    4.015E-04    2.229E-09    2.105E-01    5.977E-06    2.759E-07    4.982E-05    3.032E-02    7.927E-02    2.511E-03
 5.000E 00    1.034E-08    1.703E-01    3.884E-05    3.119E-04    1.713E-05    3.921E-02    3.425E-07    2.216E-09    5.147E-10    3.313E-03
              1.829E-06    4.782E-03    2.244E-07    4.103E-09    1.558E-02    2.762E-03    2.940E-06    1.044E-06    1.807E-04    1.594E-03
              6.402E-10    2.127E-07    1.780E-03    1.481E-05    7.057E-15    4.649E-10    5.864E-02

NET RATES    -6.463E-05   -6.633E-06   -9.313E-09    2.873E-04   -9.552E-09    1.255E-07    8.073E-08    1.226E-05    1.653E-04    3.540E-05
              6.203E-08   -2.941E-04    2.178E-07   -2.893E-06   -6.433E-07   -6.982E-05   -2.696E-09    1.887E-10    9.645E-11   -1.267E-05
             -3.029E-09    1.055E-05    1.592E-10    8.113E-10    2.090E-05   -1.486E-05    2.269E-09   -9.552E-09   -2.273E-06   -9.596E-06
             -2.758E-09    7.039E-10    4.071E-06   -2.979E-07    3.121E-08   -2.728E-12   -3.111E-05


THE REACTION RATES ARE
       3.00E-03     9.81E-03     2.44E-03     7.30E-05     1.83E-07     6.14E-06     2.74E-05     2.78E-05     9.62E-06     2.42E-11
       6.72E-05     5.45E-07     2.40E-04     3.72E-05     1.76E-04     5.82E-05     1.91E-09     1.91E-09     3.09E-06     5.84E-07
       5.84E-07     4.63E-09     4.63E-09     1.07E-05     1.93E-06     7.15E-05     8.82E-06     1.65E-06     5.77E-05     1.15E-04
       1.40E-05     1.93E-06     1.44E-06     1.08E-06     9.74E-05     8.87E-05     4.10E-05     4.70E-05     7.56E-04     7.24E-04
       1.28E-05     1.74E-05     1.07E-08     1.12E-07     1.74E-07     2.48E-09     2.60E-08     4.04E-08     1.48E-06     5.32E-07
       1.99E-07     7.72E-08     1.75E-07     2.19E-07     4.38E-08     4.73E-06     1.13E-05     4.72E-06     2.51E-06     6.40E-06
       6.40E-06     5.40E-06     5.37E-06     5.30E-07     8.79E-06     1.50E-06     1.51E-05     4.98E-07     1.08E-06     1.10E-05
       1.37E-06     1.08E-06     3.61E-04     3.13E-04     4.80E-05     6.50E-03     4.65E-06     3.64E-05     4.65E-06     2.43E-05
       7.72E-06     5.86E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
         4.750E-01    1.046E-03    1.198E-03    9.499E-03    3.086E-02    1.716E-03    9.244E-02


THE CURRENT MIXING HEIGHT IS     1186.57

THE CURRENT TEMPERATURE IS        303.00

THE CURRENT ZENITH ANGLE IS        29.68
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      TIME       NMOC        NMOC/        NOX         NO2          O3          NO2          PAR
     (LDT )      TOTAL        NOX        TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

     1600.      0.27011    56.73368    0.00476     0.94815     0.22237     0.00451     0.15570


   TIME           NO2          NO           O           O3          NO3          OH          HO2         HNO3          CO         H2O2
 INTERVAL          X           PAR         MEO2         OLE         ACO3         HCHO        RAO2         CRIG         MCRG         ETH
                  RBO2         NRAT        CRO2         GG           PAN          ARO         RARO         OPEN         PHEN         DCRB
                  APRC         PHO         NPHN         HONO         O1D          XCO          NR

 1.600E 03     4.514E-03   2.469E-04   1.959E-09   2.224E-01   7.422E-06   2.044E-07   4.628E-05   3.061E-02   8.686E-02   4.448E-03
 6.106E 00     7.703E-09   1.557E-01   4.531E-05   1.994E-04   2.309E-05   3.553E-02   1.978E-07   1.862E-09   3.549E-10   2.720E-03
               1.604E-06   5.286E-03   2.449E-07   3.187E-09   1.569E-02   2.120E-03   2.723E-06   6.197E-07   9.266E-05   1.139E-03
               3.499E-10   1.781E-07   1.944E-03   6.968E-06   5.560E-15   3.611E-10   5.691E-02

 NET RATES    -3.333E-05  -2.616E-06   1.863E-09   1.585E-04   2.872E-08  -4.627E-09  -9.602E-08   7.936E-08   1.007E-04   2.935E-05
               7.140E-10  -2.406E-04   1.430E-07  -2.004E-06   1.396E-07  -5.918E-05  -2.673E-09  -7.162E-12  -3.354E-12  -9.161E-06
              -4.641E-09   6.771E-06   4.629E-10  -1.592E-11  -9.209E-06  -9.809E-06  -2.797E-09  -6.900E-09  -1.153E-06  -6.547E-06
               3.297E-12  -2.152E-10   2.003E-06  -9.800E-08  -7.276E-12  -1.364E-12  -3.550E-05


 THE REACTION RATES ARE
      1.97E-03    8.62E-03     1.58E-03     5.52E-05     1.15E-07     4.80E-06     2.69E-05     1.48E-05     7.81E-06     9.14E-12
      5.13E-05    4.84E-07     1.37E-04     3.21E-05     1.20E-04     3.94E-05     1.07E-09     1.07E-09     1.46E-06     3.94E-07
      3.94E-07    3.34E-09     3.34E-09     6.53E-06     1.67E-06     5.93E-05     4.75E-06     5.86E-07     4.14E-05     8.28E-05
      1.01E-05    1.78E-06     8.80E-07     7.26E-07     6.54E-05     5.96E-05     3.19E-05     3.76E-05     7.30E-04     7.29E-04
      1.60E-05    1.89E-05     5.52E-09     6.72E-08     1.32E-07     1.05E-09     1.28E-08     2.52E-08     1.25E-06     4.47E-07
      1.68E-07    5.32E-08     1.21E-07     1.51E-07     3.02E-08     2.69E-06     6.42E-06     2.69E-06     9.18E-07     3.50E-06
      3.50E-06    3.44E-06     3.22E-06     4.12E-07     5.51E-06     5.68E-07     9.95E-06     1.89E-07     7.26E-07     5.82E-06
      5.87E-07    4.93E-07     2.85E-04     2.47E-04     3.78E-05     6.40E-03     3.61E-06     2.83E-05     3.61E-06     1.80E-05
      5.72E-06    5.69E-02

 THE PHOTOLYTIC RATE CONSTANTS ARE
        4.367E-01    8.971E-04    1.060E-03    8.734E-03    2.878E-02    1.280E-03    8.420E-02


 THE CURRENT MIXING HEIGHT IS     1235.00

 THE CURRENT TEMPERATURE IS        303.00

 THE CURRENT ZENITH ANGLE IS        40.64
```

```
           TIME      NMOC       NMOC/        NOX          NO2         O3          NO2         PAR
          (LDT )     TOTAL       NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

          1700.     0. 25694   65. 36827    0. 00393    0. 95661    0. 23365    0. 00376    0. 14846

   TIME          NO2         NO          O           O3          NO3         OH          HO2         HNO3        CO          H2O2
 INTERVAL        X           PAR         MEO2        OLE         ACO3        HCHO        RAO2        CRIG        MCRQ        ETH
                 RBO2        NRAT        CRO2        QQ          PAN         ARO         RARO        OPEN        PHEN        DCRB
                 APRC        PHO         NPHN        HONO        O1D         XCO         NR

 1. 700E 03   3. 760E-03  1. 706E-04  1. 729E-09  2. 337E-01  9. 593E-06  1. 374E-07  3. 852E-05  3. 142E-02  9. 406E-02  5. 989E-03
 2. 000E 01   5. 293E-09  1. 485E-01  4. 592E-05  1. 163E-04  2. 616E-05  3. 357E-02  8. 638E-08  1. 599E-09  2. 190E-10  2. 349E-03
              1. 179E-06  5. 764E-03  2. 258E-07  2. 317E-09  1. 509E-02  1. 746E-03  2. 195E-06  3. 449E-07  4. 516E-05  8. 624E-04
              1. 884E-10  1. 297E-07  2. 085E-03  3. 743E-06  3. 555E-15  2. 625E-10  5. 691E-02

 NET RATES   -1. 172E-06 -6. 742E-06  4. 956E-06  1. 515E-04 -1. 448E-07 -1. 088E-07  6. 790E-08  1. 147E-05  1. 041E-04  2. 226E-05
              7. 910E-08 -1. 036E-04 -7. 308E-09 -1. 057E-06 -1. 437E-06 -2. 773E-05 -7. 053E-09  1. 358E-09  6. 256E-10 -5. 314E-06
              9. 431E-10  7. 049E-06 -1. 002E-09 -1. 102E-08 -1. 238E-05 -5. 042E-06 -1. 004E-08 -2. 164E-08 -6. 670E-07 -3. 976E-06
             -5. 693E-09  2. 706E-08  1. 951E-06 -3. 853E-08  1. 246E-07 -9. 095E-13  0. 000E-01


 THE REACTION RATES ARE
       1. 41E-03    7. 61E-03    1. 15E-03    4. 83E-05    8. 45E-08    3. 39E-06    2. 35E-05    8. 26E-06    5. 68E-06    4. 36E-12
       4. 58E-05    5. 21E-07    7. 88E-05    2. 23E-05    7. 86E-05    2. 52E-05    5. 53E-10    5. 53E-10    5. 73E-07    2. 41E-07
       2. 41E-07    2. 55E-09    2. 55E-09    3. 79E-06    1. 52E-06    4. 64E-05    2. 41E-06    1. 77E-07    2. 90E-05    5. 80E-05
       7. 05E-06    1. 38E-06    4. 04E-07    4. 61E-07    4. 15E-05    3. 78E-05    2. 32E-05    2. 87E-05    6. 89E-04    7. 01E-04
       1. 51E-05    1. 59E-05    3. 27E-09    4. 81E-08    1. 07E-07    4. 48E-10    6. 59E-09    1. 47E-08    1. 07E-06    3. 84E-07
       1. 44E-07    3. 29E-08    7. 45E-08    9. 31E-08    1. 86E-08    1. 49E-06    3. 55E-06    1. 50E-06    3. 53E-07    1. 88E-06
       1. 88E-06    2. 17E-06    1. 95E-06    2. 50E-07    3. 22E-06    1. 86E-07    6. 48E-06    6. 20E-08    4. 62E-07    2. 96E-06
       2. 67E-07    2. 29E-07    1. 82E-04    1. 58E-04    2. 42E-05    6. 04E-03    2. 62E-06    2. 05E-05    2. 62E-06    1. 21E-05
       3. 85E-06    5. 69E-02

 THE PHOTOLYTIC RATE CONSTANTS ARE
          3. 755E-01    6. 898E-04    8. 558E-04    7. 509E-03    2. 587E-02    7. 795E-04    7. 144E-02


 THE CURRENT MIXING HEIGHT IS     1235. 00

 THE CURRENT TEMPERATURE IS        303. 00

 THE CURRENT ZENITH ANGLE IS        52. 08
```

```
           TIME      NMOC        NMOC/         NOX          NO2         O3          NO2          PAR
          (LDT )     TOTAL        NOX         TOTAL      FRACTION   (INSTANT)   (INSTANT)   (INSTANT)

          1800.     0. 24893   63. 39764    0. 00393     0. 96750    0. 24107    0. 00380     0. 14390

  TIME          NO2           NO            O             O3            NO3           OH            HO2           HNO3          CO            H2O2
INTERVAL        X             PAR           MEO2          OLE           ACO3          HCHO          RAO2          CRIG          MCRG          ETH
                RBO2          NRAT          CRO2          GG            PAN           ARO           RARO          OPEN          PHEN          DCRB
                APRC          PHO           NPHN          HONO          O1D           XCO           NR

 1. 800E 03   3. 799E-03    1. 276E-04    1. 399E-09    2. 411E-01    1. 355E-05    7. 812E-08    2. 845E-05    3. 195E-02    9. 871E-02    6. 942E-03
 1. 000E 01   3. 188E-09    1. 439E-01    3. 919E-05    7. 427E-05    2. 412E-05    3. 247E-02    3. 293E-08    1. 426E-09    1. 451E-10    2. 107E-03
              7. 092E-07    6. 092E-03    1. 663E-07    1. 411E-09    1. 415E-02    1. 541E-03    1. 485E-06    1. 717E-07    1. 732E-05    6. 798E-04
              9. 141E-11    7. 130E-08    2. 169E-03    2. 225E-06    1. 579E-15    1. 598E-10    5. 691E-02

NET RATES     3. 099E-06   -1. 169E-07    4. 405E-07    1. 003E-04    6. 083E-08   -2. 023E-08   -1. 572E-07    7. 410E-06    6. 156E-05    1. 214E-05
             -4. 341E-09   -5. 975E-05   -1. 312E-07   -5. 272E-07   -6. 129E-08   -1. 241E-05   -8. 618E-10    2. 169E-11    7. 521E-12   -3. 342E-06
             -7. 327E-09    4. 502E-06   -9. 839E-10    3. 246E-09   -1. 602E-05   -2. 531E-06   -1. 148E-08   -3. 082E-09   -3. 683E-07   -2. 466E-06
             -1. 970E-10    2. 233E-09    1. 083E-06   -1. 977E-08   -8. 574E-08   -1. 819E-12    0. 000E-01


THE REACTION RATES ARE
      1. 07E-03     6. 15E-03     8. 87E-04     5. 03E-05     6. 91E-08     1. 99E-06     1. 79E-05     4. 75E-06     3. 39E-06     2. 44E-12
      4. 84E-05     7. 44E-07     4. 36E-05     1. 21E-05     4. 59E-05     1. 39E-05     2. 86E-10     2. 86E-10     2. 08E-07     1. 59E-07
      1. 59E-07     1. 85E-09     1. 85E-09     1. 93E-06     1. 40E-06     3. 20E-05     1. 09E-06     5. 04E-08     1. 85E-05     3. 70E-05
      4. 50E-06     8. 55E-07     1. 59E-07     2. 54E-07     2. 28E-05     2. 08E-05     1. 41E-05     1. 90E-05     6. 41E-04     6. 57E-04
      1. 03E-05     1. 00E-05     2. 18E-09     4. 33E-08     9. 26E-08     2. 22E-10     4. 41E-09     9. 42E-09     9. 55E-07     3. 42E-07
      1. 28E-07     2. 18E-08     4. 93E-08     6. 17E-08     1. 23E-08     7. 47E-07     1. 78E-06     7. 58E-07     1. 31E-07     9. 14E-07
      9. 14E-07     1. 17E-06     1. 08E-06     1. 01E-07     1. 66E-06     4. 06E-08     3. 84E-06     1. 35E-08     2. 55E-07     1. 33E-06
      1. 17E-07     9. 74E-08     8. 08E-05     7. 01E-05     1. 07E-05     5. 01E-03     1. 60E-06     1. 25E-05     1. 60E-06     6. 87E-06
      2. 19E-06     5. 69E-02

THE PHOTOLYTIC RATE CONSTANTS ARE
        2. 824E-01    4. 345E-04    5. 842E-04    5. 649E-03    2. 079E-02    3. 350E-04    5. 267E-02


THE CURRENT MIXING HEIGHT IS     1235. 00

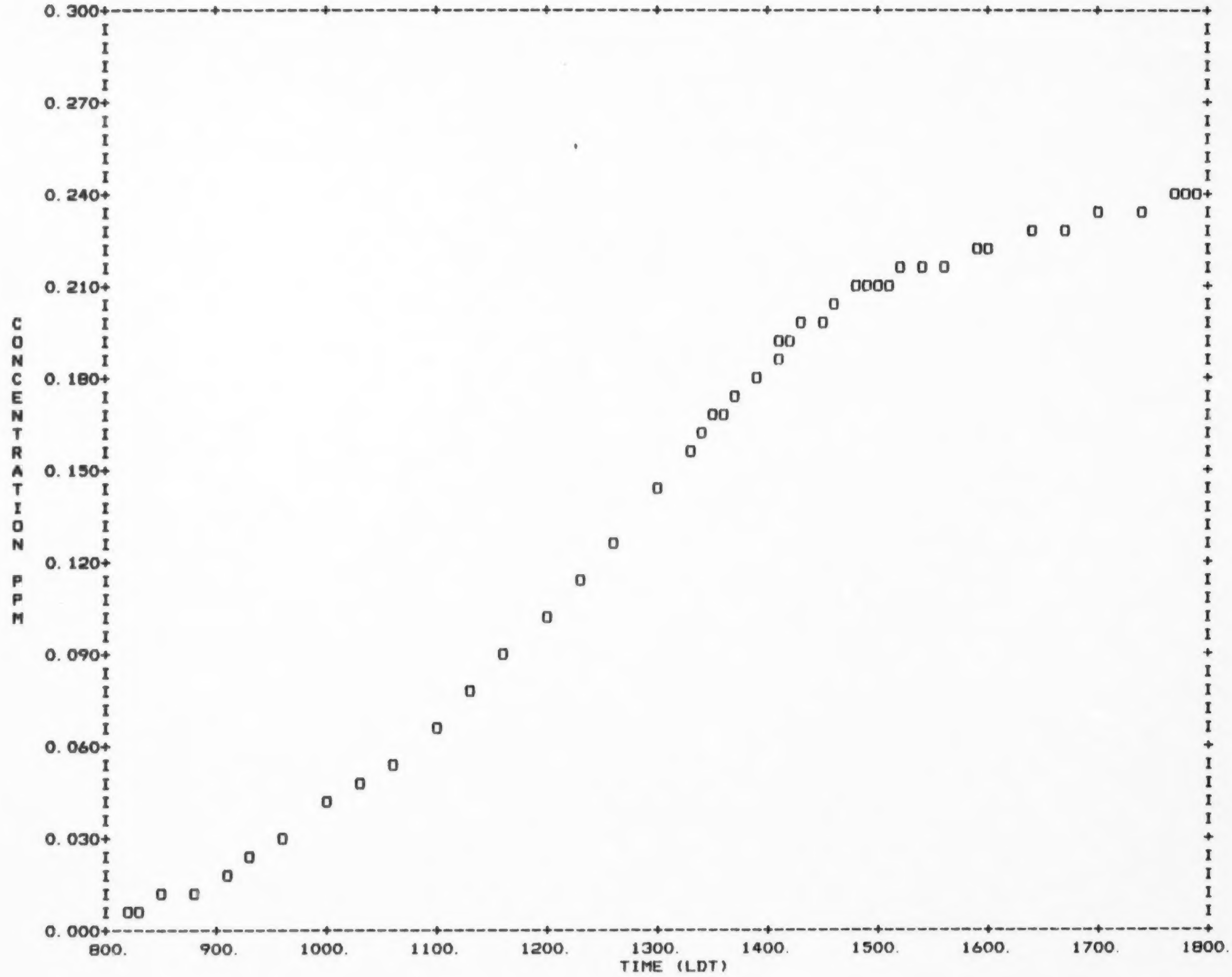
THE CURRENT TEMPERATURE IS        303. 00

THE CURRENT ZENITH ANGLE IS        63. 53
```

```
MAXIMUM O3     NOT REACHED, THE LAST ONE HOUR AVERAGE WAS 0.23761 PPM.

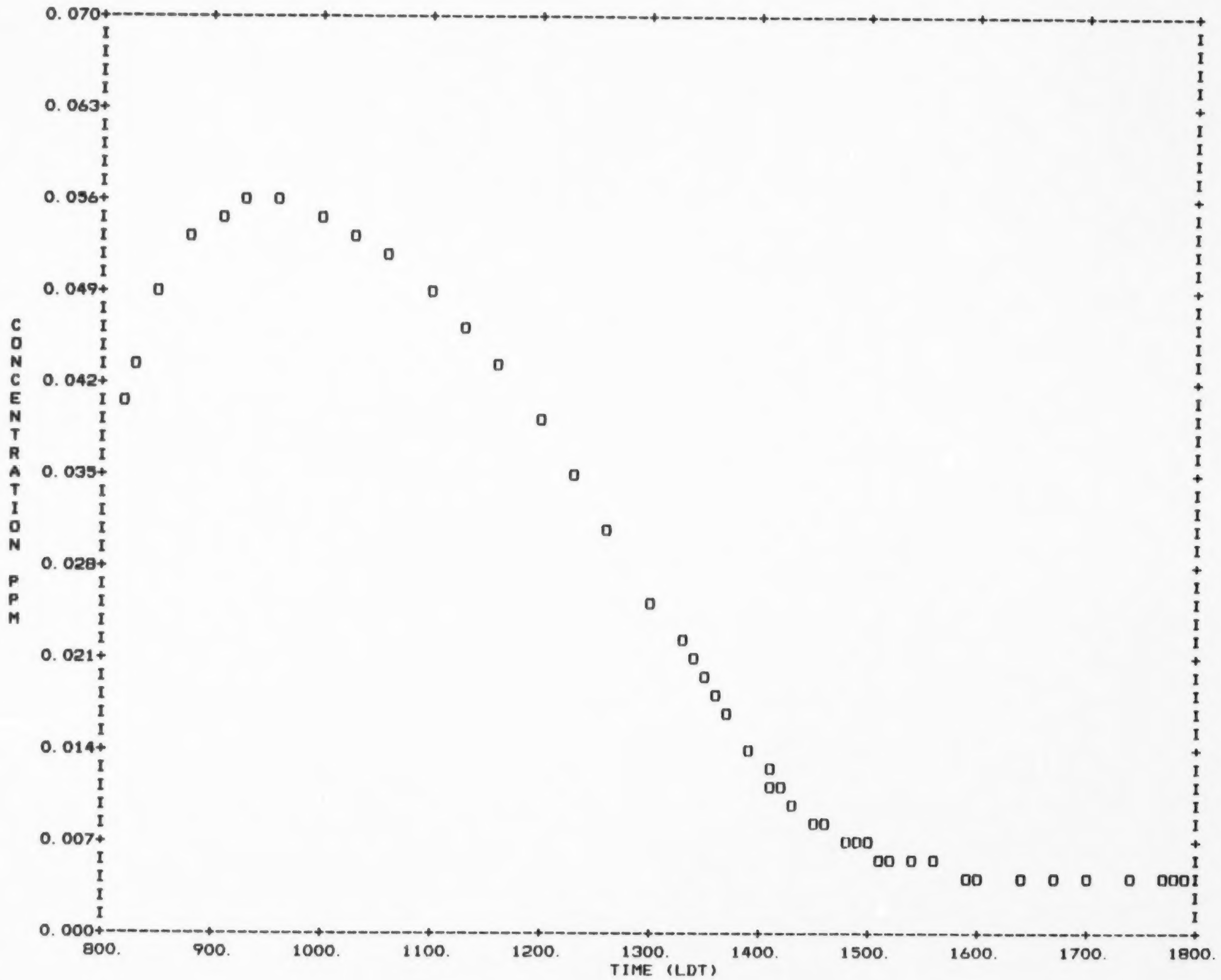
MAXIMUM ONE HOUR AVE NO2    = 0.05573 CENTERED AT  931. LDT

MAXIMUM ONE HOUR AVE PAR    = 0.55712 CENTERED AT  830. LDT
```



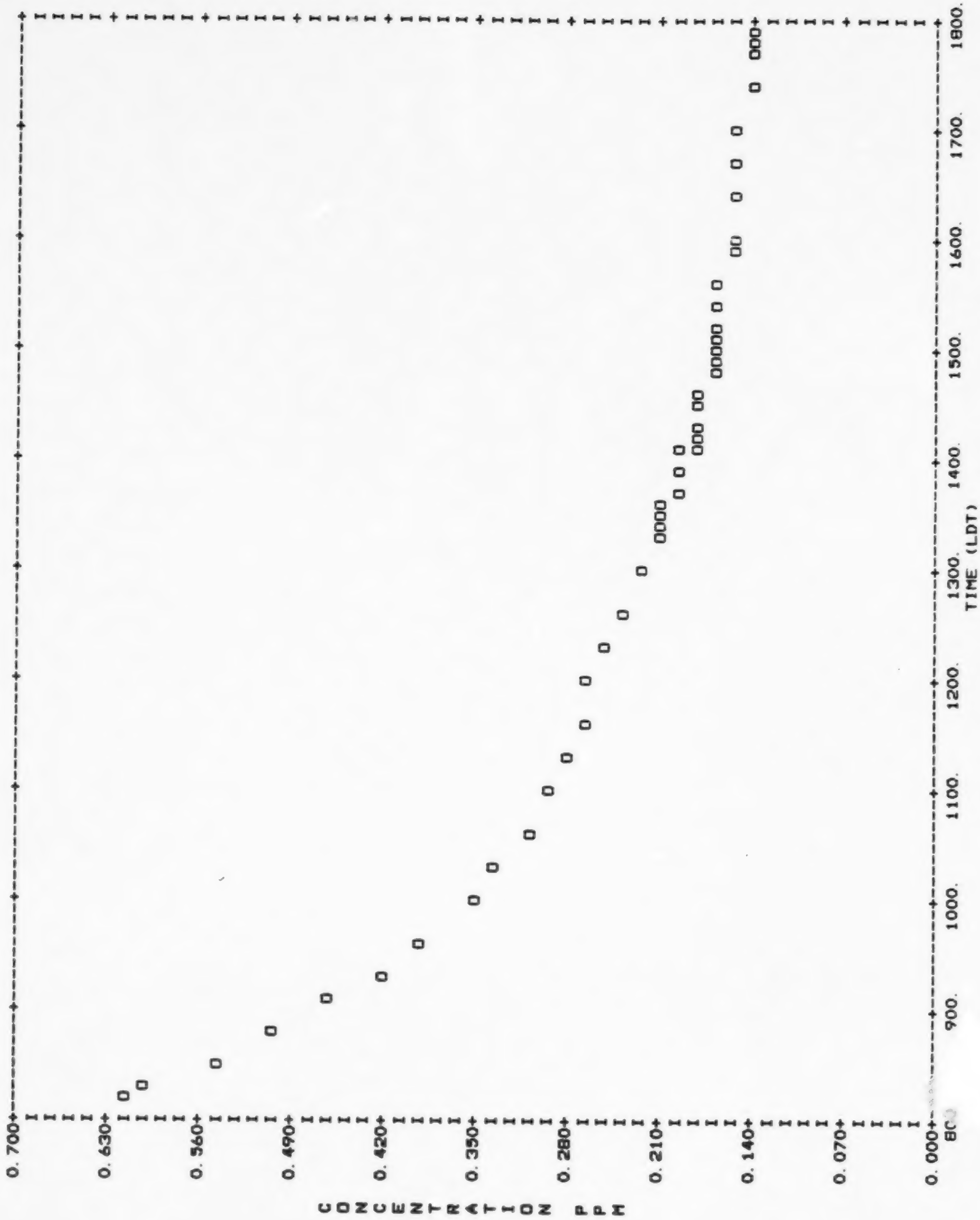
EXAMPLE 2 - TEST RUN USING EKMA/CB-3

O3 CONCENTRATION AS A FUNCTION OF TIME



EXAMPLE 2 - TEST RUN USING EKMA/CB-3

NO2 CONCENTRATION AS A FUNCTION OF TIME



EXAMPLE 2 - TEST RUN USING EKMA/CB-3

PAR CONCENTRATION AS A FUNCTION OF TIME

EXAMPLE 3

EKMA USING CBM-X

```
  1)
  2)          1         2         3         4         5         6         7
  3) 123456789012345678901234567890123456789012345678901234567890123456789012
  4)
  5) TITL
  6) EXAMPLE 3 - TEST RUN USING EKMA/CBM-X - EKMA CONTROL OPTION
  7) PLACE     39.933    75.10     5.0       1980.     6.0       24.0
  8) TEST CITY
  9) DILU      250.      1235.               1600.
 10) EMIS      -8.0      .17       .17       .17       .10       .02
 11) .02       .02       .02
 12) .35       .35       .35       .19       .03       .03       .03
 13) .07
 14) TRANS     .010      .070      .038      .040      0.0       0.0
 15) SPEC      3.
 16) O3        NO2       PAR
 17) EKMA      .171      9.5       -10.7     1.                  1.
 18) -1.       -1.       0.038     0.040     0.        0.        -50.
 19)
 20)     BLANK
```

Exhibit 5

```
****************************************
*                                      *
*   OZONE ISOPLETH PLOTTING PACKAGE    *
*      WITH OPTIONAL MECHANISMS        *
*                                      *
*              O Z I P M               *
*                                      *
*             VERSION 3.1              *
*                                      *
*           SEPTEMBER, 1985            *
*                                      *
****************************************
```

Exhibit 6

```
THE INPUTS FOR THIS RUN ARE

         TITL
         EXAMPLE 3 - TEST RUN USING EKMA/CBM-X - EKMA CONTROL OPTION
         PLACE     39.933    75.10     5.0       1980.     6.0       24.0
         TEST CITY
         DILU      250.      1235.               1600.
         EMIS      -8.0      .17       .17       .17       .10       .02
         .02       .02       .02
         .35       .35       .35       .19       .03       .03       .03
         .07
         TRANS     .010      .070      .038      .040      0.0       0.0
         SPEC      3.
         O3        NO2       PAR
         EKMA      .171      9.5       -10.7     1.                  1.
         -1.       -1.       0.038     0.040     0.        0.        -50.
```

```
EXAMPLE 3 - TEST RUN USING EKMA/CBM-X - EKMA CONTROL OPTION


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

        TEST CITY

LATITUDE     39.933

LONGITUDE    75.100

TIME ZONE    5.0

DATE         6     24    1980

TIME         800   TO    1800     LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS     INITIAL    250.      FINAL      1235.

TIMING                START      800.      STOP       1600.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME       800      900     1000     1100     1200     1300     1400     1500     1600

HEIGHT     250.0    413.6   619.2    811.8    954.3   1055.0   1129.0   1186.6   1235.0


REACTIVITY

EMISSIONS        ETH  FRACTION 0.040   OLE  FRACTION 0.030   ALD2 FRACTION 0.030

EMISSIONS        FORM FRACTION 0.020   TOL  FRACTION 0.120   XYL  FRACTION 0.100

EMISSIONS        PAR  FRACTION 0.510   NR   FRACTION 0.150

SURFACE LAYER    ETH  FRACTION 0.050   OLE  FRACTION 0.030   ALD2 FRACTION 0.160

SURFACE LAYER    FORM FRACTION 0.100   TOL  FRACTION 0.070   XYL  FRACTION 0.060

SURFACE LAYER    PAR  FRACTION 0.530   NR   FRACTION 0.000

ALOFT            ETH  FRACTION 0.060   OLE  FRACTION 0.030   ALD2 FRACTION 0.090

ALOFT            FORM FRACTION 0.060   TOL  FRACTION 0.080   XYL  FRACTION 0.070

ALOFT            PAR  FRACTION 0.610   NR   FRACTION 0.000

NO2/NOX        0.250
```

```
TRANSPORTED CONCENTRATIONS

SURFACE LAYER        OZONE   0.010      HYDROCARBON  0.038    NOX      0.000 PPM

ALOFT                OZONE   0.070      HYDROCARBON  0.040    NOX      0.000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES     HOUR           1     2     3     4     5     6     7     8

  VOC     FRACTION      0.170 0.170 0.170 0.100 0.020 0.020 0.020 0.020

  NOX     FRACTION      0.350 0.350 0.350 0.190 0.030 0.030 0.030 0.070
```

```
                  EKMA CALCULATIONS ARE PERFORMED TO ESTIMATE
                  SITE-SPECIFIC VOC CONTROL REQUIREMENTS

                  BASE YEAR OZONE                          0.171 PPM
                  BASE YEAR NMOC/NOX                       9.500
                  ANTICIPATED CHANGE IN NOX              -10.700 PERCENT
                  FUTURE OZONE TRANSPORTED ALOFT           0.062 PPM
                  FUTURE NMOC TRANSPORTED ALOFT            0.040 PPMC
                  FUTURE NOX TRANSPORTED ALOFT             0.000 PPM
                  FUTURE OZONE IN THE SURFACE LAYER        0.010 PPM
                  FUTURE NMOC IN THE SURFACE LAYER         0.038 PPMC
                  FUTURE NOX IN THE SURFACE LAYER          0.000 PPM

                  THE FOLLOWING SIMULATIONS WERE DONE.
   NMOC             NOX             RATIO             O3              TIME
 1.00000          0.10526          9.50000         0.22518          NOT MAX
 0.75940          0.07994          9.50000         0.19780          NOT MAX
 0.52394          0.05515          9.50000         0.16780          NOT MAX
 0.54906          0.05780          9.50000         0.17109          NOT MAX
 0.27453          0.05161          5.31915         0.13359          NOT MAX
 0.24660          0.05161          4.77796         0.12873          NOT MAX
 0.19641          0.05161          3.80560         0.11769          NOT MAX
 0.20691          0.05161          4.00887         0.12035          NOT MAX

                  VOC CONTROL REQUIREMENT IS  62.3 PERCENT
```

```
                    THE FOLLOWING SIMULATION WAS DONE WITH A
                     -50.00 PERCENT CHANGE IN NMOC.
    NMOC              NOX              RATIO              O3              TIME
  0.27453           0.05161          5.31915           0.13359          NOT MAX
```

EXAMPLE 4

EKMA USING CBM-X AND APPENDIX B PROCEDURES

```

         1         2         3         4         5         6         7
123456789012345678901234567890123456789012345678901234567890123456789012

TITL
EXAMPLE 4 - TEST RUN USING EKMA/CBM-X - APPENDIX B PROCEDURES
PLACE     39.933    75.10     5.0       1980.     6.0       24.0
TEST CITY
DILU      250.      1235.               1600.
EMIS      -8.0      .17       .17       .17       .10       .02
.02       .02       .02
.35       .35       .35       .19       .03       .03       .03
.07
TRANS     .010      .070      .080      .070      0.0       0.0
SPEC      3.
O3        NO2       PAR
EKMA      .171      9.5       -10.7     1.
-1.       -1.       -.32      0.000     0.        0.

    BLANK
```

Exhibit 7

```
****************************************
*                                      *
*   OZONE ISOPLETH PLOTTING PACKAGE    *
*      WITH OPTIONAL MECHANISMS        *
*                                      *
*              O Z I P M               *
*                                      *
*             VERSION 3.1              *
*                                      *
*           SEPTEMBER, 1985            *
*                                      *
****************************************
```

Exhibit 8

```
THE INPUTS FOR THIS RUN ARE

         TITL
         EXAMPLE 4 - TEST RUN USING EKMA/CBM-X - APPENDIX B PROCEDURES
         PLACE     39.933    75.10     5.0       1980.     6.0       24.0
         TEST CITY
         DILU      250.      1235.               1600.
         EMIS      -8.0      .17       .17       .17       .10       .02
         .02       .02       .02
         .35       .35       .35       .19       .03       .03       .03
         .07
         TRANS     .010      .070      .080      .070      0.0       0.0
         SPEC      3.
         O3        NO2       PAR
         EKMA      .171      9.5       -10.7     1.
         -1.       -1.       -.32      0.000     0.        0.
```

```
EXAMPLE 4 - TEST RUN USING EKMA/CBM-X - APPENDIX B PROCEDURES

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

        TEST CITY

LATITUDE     39.933

LONGITUDE    75.100

TIME ZONE    5.0

DATE         6     24    1980

TIME         800   TO    1800     LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS     INITIAL   250.     FINAL      1235.

TIMING                START     800.     STOP       1600.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME       800      900     1000     1100     1200     1300     1400     1500     1600

HEIGHT     250.0    413.6   619.2    811.8    954.3    1055.0   1129.0   1186.6   1235.0


REACTIVITY

EMISSIONS        ETH  FRACTION 0.040   OLE  FRACTION 0.030   ALD2 FRACTION 0.030

EMISSIONS        FORM FRACTION 0.020   TOL  FRACTION 0.120   XYL  FRACTION 0.100

EMISSIONS        PAR  FRACTION 0.510   NR   FRACTION 0.150

SURFACE LAYER    ETH  FRACTION 0.050   OLE  FRACTION 0.030   ALD2 FRACTION 0.160

SURFACE LAYER    FORM FRACTION 0.100   TOL  FRACTION 0.070   XYL  FRACTION 0.060

SURFACE LAYER    PAR  FRACTION 0.530   NR   FRACTION 0.000

ALOFT            ETH  FRACTION 0.060   OLE  FRACTION 0.030   ALD2 FRACTION 0.090

ALOFT            FORM FRACTION 0.060   TOL  FRACTION 0.080   XYL  FRACTION 0.070

ALOFT            PAR  FRACTION 0.610   NR   FRACTION 0.000

NO2/NOX       0.250
```

```
TRANSPORTED CONCENTRATIONS

SURFACE LAYER        OZONE   0.010      HYDROCARBON  0.080     NOX      0.000 PPM

ALOFT                OZONE   0.070      HYDROCARBON  0.070     NOX      0.000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES     HOUR          1     2     3     4     5     6     7     8

  VOC      FRACTION     0.170 0.170 0.170 0.100 0.020 0.020 0.020 0.020

  NOX      FRACTION     0.350 0.350 0.350 0.190 0.030 0.030 0.030 0.070
```

```
EKMA CALCULATIONS ARE PERFORMED TO ESTIMATE

SITE-SPECIFIC VOC CONTROL REQUIREMENTS


BASE YEAR OZONE                            0.171 PPM

BASE YEAR NMOC/NOX                         9.500

ANTICIPATED CHANGE IN NOX                -10.700 PERCENT

FUTURE OZONE TRANSPORTED ALOFT             0.062 PPM

FUTURE NMOC TRANSPORTED ALOFT              0.000 PPMC

FUTURE NOX TRANSPORTED ALOFT               0.000 PPM

MEDIAN CONTRIBUTION FACTOR FOR NMOC        0.320

MEDIAN CONTRIBUTION FACTOR FOR NOX         0.000

ADJUSTED NMOC/NOX                          6.460

FUTURE OZONE IN THE SURFACE LAYER          0.010 PPM

FUTURE NMOC IN THE SURFACE LAYER           0.048 PPMC

FUTURE NOX IN THE SURFACE LAYER            0.000 PPM



THE FOLLOWING SIMULATIONS WERE DONE.

  NMOC           NOX           RATIO           O3           TIME

1.00000        0.10526       9.50000       0.22839        NOT MAX

0.74871        0.07881       9.50000       0.19963        NOT MAX

0.49863        0.05249       9.50000       0.16735        NOT MAX

0.52692        0.05547       9.50000       0.17118        NOT MAX

0.35831        0.05547       6.46000       0.17232        NOT MAX

0.35557        0.05504       6.46000       0.17183        NOT MAX

0.17779        0.04915       3.61702       0.10630        NOT MAX

0.20071        0.04915       4.08337       0.11274        NOT MAX

0.22653        0.04915       4.60868       0.11892        NOT MAX

0.23104        0.04915       4.70057       0.11992        NOT MAX


VOC CONTROL REQUIREMENT IS  35.0 PERCENT
```

EXAMPLE 5

ISOP USING OPTIONAL MECHANISM

```

         1         2         3         4         5         6         7
123456789012345678901234567890123456789012345678901234567890123456789012

PLOT                           8.        5. 6
MECH        111.     15.      8.
1.        8.        9.        21.       26.       30.       38.
39.       47.       61.       67.       69.       71.       81.
105.
ETH       OLE       ALD2      FORM      TOL       XYL       PAR
NR
2.        2.        2.        1.        7.        8.        1.
1.
NO2               1     NO         O                   1.
O                 2     O3                             4440000.    -690.
O3   NO           3     NO2                            26. 6       1430.
O    NO2          4     NO                             13800.
O    NO2          5     NO3                            2320.       -600.
O    NO           6     NO2                            3120.       -411.
NO2  O3           7     NO3                            0. 0474     2450.
O3                8     O1D                            1. 16
O3                9     O                              0. 042
O1D              10     O                                4. 29E10  -100.
O1D              11 2.  OH                               6. 52E09
O3   OH          12     HO2                            100.         940.
O3   HO2         13     OH                             3. 0         580.
NO3  NO          14 2.  NO2                            28100.      -250.
NO3  NO2         15     NO         NO2                 0. 59       1231.
NO3  NO2         16     N2O5                           1780.         60.
N2O5             17 2.  HNO3                           . 038
N2O5             18     NO3        NO2                 3. 12      10840.
NO   NO2         19 2.  HNO2                             3. 2E-7
HNO2 HNO2        20     NO         NO2                   1. 5E-5
HNO2             21     NO         OH                  0. 18
NO2  OH          22     HNO3                           16300.      -560.
NO   OH          23     HNO2                           9770.       -427.
HO2  NO          24     OH         NO2                 12300.      -240.
NO   NO          25 2.  NO2                            . 000152    -530.
H2O2             26 2.  OH                             0. 0014
OH   H2O2        27     HO2                            2520.        187.
OH   HNO2        28     NO2                            9770.
OH   HNO3        29     NO3                            192.        -778.
NO3             300. 85 NO2  0. 85 O     0. 15 NO      30. 6
HO2  HO2         31     H2O2                           4144.      -1150.
HO2  HO2         32     H2O2                           4360.      -5800.
HO2  NO2         33     PNA                            1630.       -617.
PNA              34     HO2        NO2                 5. 12      10420.
OH   CO          35     HO2                            400.
FORM HO2         36     FROX                           14. 8
FORM OH          37     HO2        CO                  15000.
FORM             38 2.  HO2        CO                  1. 1
FORM             39     CO                             1. 06
FORM O           40     OH         HO2         CO      237.        1550.
FORM NO3         41     HNO3       HO2         CO      0. 93
FROX NO          42     NO2        HO2                 10400.
FROX             43     FORM       HO2                 90.
ALD2 O           44     C2O3       OH                  636.         986.
ALD2 OH          45     C2O3                           24000.      -250.
ALD2 NO3         46     C2O3       HNO3                3. 7
ALD2             47     MEO2       HO2         CO      1. 11
```

Exhibit 9

```
(        61)  ALD2   HO2          48      MEO2          FORM                  5.
(        62)  C2O3   NO           49      MEO2          NO2                   16500.        -250.
(        63)  C2O3   NO2          50      PAN                                 9000.         -250.
(        64)  PAN                 51      C2O3          NO2                   0.0222       14000.
(        65)  MEO2   NO2          52      MPNA                                6000.         -735.
(        66)  MPNA                53      MEO2          NO2                   92.          10400.
(        67)  MEO2   NO           54      MEO           NO2                   11000.        -180.
(        68)  MEO    NO           55      MNIT                                44400.        -200.
(        69)  MEO    NO           56      FORM          HO2           NO      1920.
(        70)  MEO    NO2          57      MEN3                                22200.
(        71)  MEO                 58      FORM          HO2                   394000.       1313.
(        72)  MEN3   OH           59      FORM          NO2                   2220.          360.
(        73)  MNIT   OH           60      FORM          NO                    2370.          340.
(        74)  MNIT                61      MEO           NO                    0.3
(        75)  MEO2   MEO2         620.70  MEO    0.65   FORM                  503.          -220.
(        76)  MEO2   C2O3         63      MEO           MEO2                  4400.
(        77)  C2O3   C2O3         642.    MEO2                                3700.
(        78)  MEO2   HO2          65                                          8900.        -1300.
(        79)  C2O3   HO2          66                                          9600.
(        80)  AONE                67      MEO2          C2O3                  0.00004
(        81)  AONE   OH           68      XO2           FORM          C2O3    580.
(        82)  GLY                 691.79  CO     0.21   FORM   0.19   HO2     0.0075
(        83)  GLY    OH           70      HO2    2.     CO                    15000.
(        84)  MGLY                71      C2O3          HO2           CO      0.02
(        85)  MGLY   OH           72      XO2           C2O3                  26000.
(        86)  OH                  73      MEO2                                21.
(        87)  PAR    OH           740.92  XO2 *  0.79   ROR    0.13   HO2     1150.0
(        88)  0.13   ALD2   -0.13 PAR     0.067  XO2N
(        89)  ROR    NO2          75                                          22000.
(        90)  ROR                 760.38  KET *  0.38   HO2    0.62   AONE    390000.
(        91)  0.62   D      -1.24 PAR
(        92)  ROR                 77      ALD2          D     -1.0    PAR     90000.        7000.
(        93)  D      PAR          78      XO2 *         HO2    0.7    AONE    10000.
(        94)  0.3    ALD2   -1.7  PAR
(        95)  D      KET          79      C2O3    -1.0  PAR                   10000.
(        96)  XO2    NO           80      NO2                                 12000.
(        97)  KET                 81      C2O3*         XO2           HO2     .0003
(        98)         ALD2   -3.0  PAR
(        99)  O      OLE          820.95  ALD2*  0.30   HO2    0.15   XO2     5920.          324.
(       100)  0.15   CO     0.05  MEO2    0.05   C2O3  -0.35 PAR
(       101)  OH     OLE          83      MEO2          ALD2  -1.0    PAR     42000.        -537.
(       102)  O3     OLE          840.5   ALD2*  0.516  FORM   0.3    MCRG    0.018         1897.
(       103)  0.3    CRIG   0.212 CO      0.136  HO2    0.144  MEO2   -1.0    PAR   0.08  OH
(       104)  NO3    OLE          850.91  XO2    0.91   HO2    0.09   XO2N    11.4
(       105)  O      ETH          86      MEO2          HO2           CO      1080.          800.
(       106)  OH     ETH          87      MEO2          FORM                  12000.        -382.
(       107)  O3     ETH          88      FORM*  0.37   CRIG   0.37   CO      0.0027        2840.
(       108)  0.13   HO2
(       109)  CRIG   NO           89      FORM          NO2                   10000.
(       110)  CRIG   NO2          90      FORM          NO3                   1000.
(       111)  CRIG                91                                          120.
(       112)  CRIG   FORM         92                                          30.
(       113)  CRIG   ALD2         93                                          30.
(       114)  MCRG   NO           94      ALD2          NO2                   10000.
(       115)  MCRG   NO2          95      ALD2          NO3                   1000.
(       116)  MCRG                96                                          120.
(       117)  MCRG   FORM         97                                          30.
(       118)  MCRG   ALD2         98                                          30.
(       119)  TOL    OH           99      HO2 *  0.64   XO2    1.13   GLY     9750.
(       120)  0.56   MGLY   0.36  PHEN    0.36   PAR    0.077 BZA
(       121)  PHEN  NO3       100     PHO         HNO3                14000.
(       122)  BZA   OH        101     BZO2                            20000.
(       123)  BZO2  NO2       102     PBZN                            2500.
(       124)  BZO2  NO        103     XO2 *       PHO          CO     3700.
(       125)        NO2
(       126)  PBZN            104     BZO2        NO2                 .022      14000.
(       127)  BZA             105                                     .004
(       128)  PHO   NO2       106                                     20000.
(       129)  XYL   OH        107     HO2 * 0.72  XO2    0.67  QLY    36000.
(       130)  1.33  MGLY  0.28  PHEN  0.56  PAR   0.06   TLA
(       131)  TLA   OH        108     XO2         PHO    2.    PAR    20000.
(       132)  XO2   HO2       109                                     10000.
(       133)  OH              110     HO2                             88.
(       134)  NR              111     NR                              1.
(       135)  ZENITH     4.
(       136)  8.          0.00466   0.00455   0.00416    0.00353   0.00277   0.00192
(       137)     0.00111 0.000476  0.000210  0.000112
(       138)  39.         0.00376   0.00375   0.00370    0.00360   0.00346   0.00326
(       139)     0.00299  0.00259   0.00229   0.00218
(       140)  38.         0.00271   0.00270   0.00261    0.00248   0.00228   0.00201
(       141)     0.00164  0.00125  0.000915  0.000690
(       142)  47.        0.000644  0.000624  0.000605   0.000540  0.000473  0.000374
(       143)    0.000274 0.000191  0.000108  0.000054
(       144)  TITL
(       145)  EXAMPLE 5 - TEST RUN USING EKMA/CBM-X (STOICHIOMETRIC COEFF)
(       146)  PLACE     39.933    75.10      5.0       1980.     6.0       24.0
(       147)  TEST CITY
(       148)  DILU      250.      1235.                1600.
(       149)  REAC      8.0
(       150)  0.04      0.03      0.03       0.02      0.12      0.10      0.51
(       151)  .15
(       152)  EMIS      -8.0      .17        .17       .17       .10       .02
(       153)  .02       .02       .02
(       154)  .35       .35       .35        .19       .03       .03       .03
(       155)  .07
(       156)  TRANS     .010      .070       -8.       -8.       0.0       0.0
(       157)  .038      .05       .03        .16       .10       .07       .06
(       158)  .53       0.
(       159)  .040      .06       .03        .09       .06       .08       .07
(       160)  .61       0.
(       161)  SPEC      3.
(       162)  O3        NO2       PAR
(       163)  CALC      1.1       .12
(       164)  ISOP                                     1.
(       165)
(       166)      BLANK
```

```
**************************************
*                                    *
*  OZONE ISOPLETH PLOTTING PACKAGE   *
*     WITH OPTIONAL MECHANISMS       *
*                                    *
*            O Z I P M               *
*                                    *
*           VERSION 3.1              *
*                                    *
*         SEPTEMBER, 1985            *
*                                    *
**************************************
```

Exhibit 10

THE INPUTS FOR THIS RUN ARE

```
PLOT                                         8.             5. 6
MECH             111.          15.           8.
1.             8.            9.              21.            26.         30.           38.
39.            47.           61.             67.            69.         71.           81.
105.
ETH            OLE           ALD2            FORM           TOL         XYL           PAR
NR
2.             2.            2.              1.             7.          8.            1.
1.
NO2                     1          NO              O                          1.
O                       2          O3                                         4440000.     -690.
O3      NO              3          NO2                                        26. 6        1430.
O       NO2             4          NO                                         13800.
O       NO2             5          NO3                                        2320.        -600.
O       NO              6          NO2                                        3120.        -411.
NO2     O3              7          NO3                                        0. 0474      2450.
O3                      8          O1D                                        1. 16
O3                      9          O                                          0. 042
O1D                     10         O                                             4. 29E10  -100.
O1D                     11 2.      OH                                             6. 52E09
O3      OH              12         HO2                                        100.          940.
O3      HO2             13         OH                                         3. 0          580.
NO3     NO              14 2.      NO2                                        28100.       -250.
NO3     NO2             15         NO              NO2                        0. 59        1231.
NO3     NO2             16         N2O5                                       1780.          60.
N2O5                    17 2.      HNO3                                       .038
N2O5                    18         NO3             NO2                        3. 12       10840.
NO      NO2             19 2.      HNO2                                           3. 2E-7
HNO2    HNO2            20         NO              NO2                            1. 5E-5
HNO2                    21         NO              OH                         0. 18
NO2     OH              22         HNO3                                       16300.       -560.
NO      OH              23         HNO2                                       9770.        -427.
HO2     NO              24         OH              NO2                        12300.       -240.
NO      NO              25 2.      NO2                                        .000152      -530.
H2O2                    26 2.      OH                                         0. 0014
OH      H2O2            27         HO2                                        2520.         187.
OH      HNO2            28         NO2                                        9770.
OH      HNO3            29         NO3                                        192.         -778.
NO3                     300. 85    NO2     0. 85   O        0. 15    NO       30. 6
HO2     HO2             31         H2O2                                       4144.       -1150.
HO2     HO2             32         H2O2                                       4360.       -5800.
HO2     NO2             33         PNA                                        1630.        -617.
PNA                     34         HO2             NO2                        5. 12       10420.
OH      CO              35         HO2                                        400.
FORM    HO2             36         FROX                                       14. 8
FORM    OH              37         HO2             CO                         15000.
FORM                    38 2.      HO2             CO                         1. 1
FORM                    39         CO                                         1. 06
FORM    O               40         OH              HO2              CO        237.         1550.
```

```
THE INPUTS FOR THIS RUN ARE

FORM  NO3        41     HNO3        HO2         CO     0.93
FROX  NO         42     NO2         HO2                10400.
FROX             43     FORM        HO2                90.
ALD2  O          44     C203        OH                 636.       986.
ALD2  OH         45     C203                           24000.    -250.
ALD2  NO3        46     C203        HNO3               3.7
ALD2             47     MEO2        HO2         CO     1.11
ALD2  HO2        48     MEO2        FORM               5.
C203  NO         49     MEO2        NO2                16500.    -250.
C203  NO2        50     PAN                            9000.     -250.
PAN              51     C203        NO2                0.0222   14000.
MEO2  NO2        52     MPNA                           6000.     -735.
MPNA             53     MEO2        NO2                92.      10400.
MEO2  NO         54     MEO         NO2                11000.    -180.
MEO   NO         55     MNIT                           44400.    -200.
MEO   NO         56     FORM        HO2         NO     1920.
MEO   NO2        57     MEN3                           22200.
MEO              58     FORM        HO2                394000.   1313.
MEN3  OH         59     FORM        NO2                2220.      360.
MNIT  OH         60     FORM        NO                 2370.      340.
MNIT             61     MEO         NO                 0.3
MEO2  MEO2       620.70 MEO   0.65  FORM               503.      -220.
MEO2  C203       63     MEO         MEO2               4400.
C203  C203       642.   MEO2                           3700.
MEO2  HO2        65                                    8900.    -1300.
C203  HO2        66                                    9600.
AONE             67     MEO2        C203               0.00004
AONE  OH         68     XO2         FORM        C203   580.
QLY              691.79 CO     0.21 FORM  0.19  HO2    0.0075
QLY   OH         70     HO2   2.    CO                 15000.
MQLY             71     C203        HO2         CO     0.02
MQLY  OH         72     XO2         C203               26000.
OH               73     MEO2                           21.
PAR   OH         740.92 XO2 * 0.79  ROR   0.13  HO2    1150.0
0.13  ALD2 -0.13 PAR    0.067 XO2N
ROR   NO2        75                                    22000.
ROR              760.38 KET * 0.38  HO2   0.62  AONE   390000.
0.62  D    -1.24 PAR
ROR              77     ALD2        D     -1.0  PAR    90000.    7000.
D     PAR        78     XO2 *       HO2   0.7   AONE   10000.
0.3   ALD2 -1.7   PAR
D     KET        79     C203  -1.0  PAR                10000.
XO2   NO         80     NO2                            12000.
KET              81     C203*       XO2         HO2    .0003
      ALD2 -3.0   PAR
O     OLE        820.95 ALD2* 0.30  HO2   0.15  XO2    5920.      324.
0.15  CO   0.05   MEO2  0.05  C203  -0.35 PAR
OH    OLE        83     MEO2        ALD2  -1.0  PAR    42000.    -537.
O3    OLE        840.5  ALD2* 0.516 FORM  0.3   MCRG   0.018     1897.
0.3   CRIG 0.212 CO     0.136 HO2   0.144 MEO2  -1.0  PAR    0.08   OH
```

THE INPUTS FOR THIS RUN ARE

```
NO3  OLE         850.91 XO2  0.91  HO2   0.09  XO2N  11.4
O    ETH         86     MEO2       HO2         CO    1080.       800.
OH   ETH         87     MEO2       FORM              12000.     -382.
O3   ETH         88     FORM* 0.37 CRIG  0.37  CO    0.0027     2840.
0.13 HO2
CRIG NO          89     FORM       NO2               10000.
CRIG NO2         90     FORM       NO3               1000.
CRIG             91                                  120.
CRIG FORM        92                                  30.
CRIG ALD2        93                                  30.
MCRG NO          94     ALD2       NO2               10000.
MCRG NO2         95     ALD2       NO3               1000.
MCRG             96                                  120.
MCRG FORM        97                                  30.
MCRG ALD2        98                                  30.
TOL  OH          99     HO2 * 0.64 XO2   1.13  GLY   9750.
0.56 MGLY  0.36  PHEN   0.36  PAR  0.077 BZA
PHEN NO3         100    PHO        HNO3              14000.
BZA  OH          101    BZO2                         20000.
BZO2 NO2         102    PBZN                         2500.
BZO2 NO          103    XO2 *      PHO         CO    3700.
     NO2
PBZN             104    BZO2       NO2               .022       14000.
BZA              105                                 .004
PHO  NO2         106                                 20000.
XYL  OH          107    HO2 * 0.72 XO2   0.67  GLY   36000.
1.33 MGLY  0.28  PHEN   0.56  PAR  0.06  TLA
TLA  OH          108    XO2        PHO   2.    PAR   20000.
XO2  HO2         109                                 10000.
OH               110    HO2                          88.
NR               111    NR                           1.
ZENITH         4.
8.             0.00466   0.00455   0.00416   0.00353   0.00277   0.00192
  0.00111     0.000476  0.000210  0.000112
39.            0.00376   0.00375   0.00370   0.00360   0.00346   0.00326
  0.00299      0.00259   0.00229   0.00218
38.            0.00271   0.00270   0.00261   0.00248   0.00228   0.00201
  0.00164      0.00125  0.000915  0.000690
47.           0.000644  0.000624  0.000605  0.000540  0.000473  0.000374
 0.000274     0.000191  0.000108  0.000054
TITL
EXAMPLE 5 - TEST RUN USING EKMA/CBM-X (STOICHIOMETRIC COEFF)
PLACE     39.933    75.10     5.0       1980.     6.0       24.0
TEST CITY
DILU      250.      1235.               1600.
REAC      8.0
0.04      0.03      0.03      0.02      0.12      0.10      0.51
.15
EMIS      -8.0      .17       .17       .17       .10       .02
.02       .02       .02
```

```
THE INPUTS FOR THIS RUN ARE
          .35       .35       .35       .19       .03       .03       .03
          .07
          TRANS     .010      .070      -8.       -8.       0.0       0.0
          .038      .05       .03       .16       .10       .07       .06
          .53       0.
          .040      .06       .03       .09       .06       .08       .07
          .61       0.
          SPEC      3.
          03        NO2       PAR
          CALC      1.1       .12
          ISOP                                    1.
```

```
THE REACTIONS                                                         RATE CONSTANT  ACT. ENERGY(K)
  1      NO2                  =    NO    +    O                        1.000E 00      0.000E-01
  2      O                    =    O3                                  4.440E 06     -6.900E 02
  3      O3    +    NO        =    NO2                                 2.660E 01      1.430E 03
  4      O     +    NO2       =    NO                                  1.380E 04      0.000E-01
  5      O     +    NO2       =    NO3                                 2.320E 03     -6.000E 02
  6      O     +    NO        =    NO2                                 3.120E 03     -4.110E 02
  7      NO2   +    O3        =    NO3                                 4.740E-02      2.450E 03
  8      O3                   =    O1D                                 1.160E 00      0.000E-01
  9      O3                   =    O                                   4.200E-02      0.000E-01
 10      O1D                  =    O                                   4.290E 10     -1.000E 02
 11      O1D                  =  2 OH                                  6.520E 09      0.000E-01
 12      O3    +    OH        =    HO2                                 1.000E 02      9.400E 02
 13      O3    +    HO2       =    OH                                  3.000E 00      5.800E 02
 14      NO3   +    NO        =  2 NO2                                 2.810E 04     -2.500E 02
 15      NO3   +    NO2       =    NO    +    NO2                      5.900E-01      1.231E 03
 16      NO3   +    NO2       =    N2O5                                1.780E 03      6.000E 01
 17      N2O5                 =  2 HNO3                                3.800E-02      0.000E-01
 18      N2O5                 =    NO3   +    NO2                      3.120E 00      1.084E 04
 19      NO    +    NO2       =  2 HNO2                                3.200E-07      0.000E-01
 20      HNO2  +    HNO2      =    NO    +    NO2                      1.500E-05      0.000E-01
 21      HNO2                 =    NO    +    OH                       1.800E-01      0.000E-01
 22      NO2   +    OH        =    HNO3                                1.630E 04     -5.600E 02
 23      NO    +    OH        =    HNO2                                9.770E 03     -4.270E 02
 24      HO2   +    NO        =    OH    +    NO2                      1.230E 04     -2.400E 02
 25      NO    +    NO        =  2 NO2                                 1.520E-04     -5.300E 02
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THE REACTIONS                                                          RATE CONSTANT  ACT. ENERGY(K)
 26     H2O2             =     2 OH                                     1.400E-03      0.000E-01
 27     OH   +   H2O2    =       HO2                                    2.520E 03      1.870E 02
 28     OH   +   HNO2    =       NO2                                    9.770E 03      0.000E-01
 29     OH   +   HNO3    =       NO3                                    1.920E 02     -7.780E 02
 30     NO3              =  0.85 NO2  + 0.85 O    + 0.15 NO             3.060E 01      0.000E-01
 31     HO2  +   HO2     =       H2O2                                   4.144E 03     -1.150E 03
 32     HO2  +   HO2     =       H2O2                                   4.360E 03     -5.800E 03
 33     HO2  +   NO2     =       PNA                                    1.630E 03     -6.170E 02
 34     PNA              =       HO2  +    NO2                          5.120E 00      1.042E 04
 35     OH   +   CO      =       HO2                                    4.000E 02      0.000E-01
 36     FORM +   HO2     =       FROX                                   1.480E 01      0.000E-01
 37     FORM +   OH      =       HO2  +    CO                           1.500E 04      0.000E-01
 38     FORM             =     2 HO2  +    CO                           1.100E 00      0.000E-01
 39     FORM             =       CO                                     1.060E 00      0.000E-01
 40     FORM +   O       =       OH   +    HO2   +    CO                2.370E 02      1.550E 03
 41     FORM +   NO3     =       HNO3 +    HO2   +    CO                9.300E-01      0.000E-01
 42     FROX +   NO      =       NO2  +    HO2                          1.040E 04      0.000E-01
 43     FROX             =       FORM +    HO2                          9.000E 01      0.000E-01
 44     ALD2 +   O       =       C2O3 +    OH                           6.360E 02      9.860E 02
 45     ALD2 +   OH      =       C2O3                                   2.400E 04     -2.500E 02
 46     ALD2 +   NO3     =       C2O3 +    HNO3                         3.700E 00      0.000E-01
 47     ALD2             =       MEO2 +    HO2   +    CO                1.110E 00      0.000E-01
 48     ALD2 +   HO2     =       MEO2 +    FORM                         5.000E 00      0.000E-01
 49     C2O3 +   NO      =       MEO2 +    NO2                          1.650E 04     -2.500E 02
 50     C2O3 +   NO2     =       PAN                                    9.000E 03     -2.500E 02
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THE REACTIONS                                                                       RATE CONSTANT  ACT. ENERGY(K)

 51      PAN                      =       C2O3  +     NO2                           2.220E-02      1.400E 04

 52      MEO2  +    NO2           =       MPNA                                      6.000E 03     -7.350E 02

 53      MPNA                     =       MEO2  +     NO2                           9.200E 01      1.040E 04

 54      MEO2  +    NO            =       MEO   +     NO2                           1.100E 04     -1.800E 02

 55      MEO   +    NO            =       MNIT                                      4.440E 04     -2.000E 02

 56      MEO   +    NO            =       FORM  +     HO2   +     NO                1.920E 03      0.000E-01

 57      MEO   +    NO2           =       MEN3                                      2.220E 04      0.000E-01

 58      MEO                      =       FORM  +     HO2                           3.940E 05      1.313E 03

 59      MEN3  +    OH            =       FORM  +     NO2                           2.220E 03      3.600E 02

 60      MNIT  +    OH            =       FORM  +     NO                            2.370E 03      3.400E 02

 61      MNIT                     =       MEO   +     NO                            3.000E-01      0.000E-01

 62      MEO2  +    MEO2          =   0.7 MEO   + 0.65 FORM                         5.030E 02     -2.200E 02

 63      MEO2  +    C2O3          =       MEO   +     MEO2                          4.400E 03      0.000E-01

 64      C2O3  +    C2O3          =     2 MEO2                                      3.700E 03      0.000E-01

 65      MEO2  +    HO2           =                                                 8.900E 03     -1.300E 03

 66      C2O3  +    HO2           =                                                 9.600E 03      0.000E-01

 67      AONE                     =       MEO2  +     C2O3                          4.000E-05      0.000E-01

 68      AONE  +    OH            =       XO2   +     FORM  +     C2O3              5.800E 02      0.000E-01

 69      GLY                      =  1.79 CO    + 0.21 FORM + 0.19 HO2              7.500E-03      0.000E-01

 70      GLY   +    OH            =       HO2   +   2 CO                            1.500E 04      0.000E-01

 71      MGLY                     =       C2O3  +     HO2   +     CO                2.000E-02      0.000E-01

 72      MGLY  +    OH            =       XO2   +     C2O3                          2.600E 04      0.000E-01

 73      OH                       =       MEO2                                      2.100E 01      0.000E-01

 74      PAR   +    OH            =  0.92 XO2   + 0.79 ROR  + 0.13 HO2  + 0.13 ALD2 1.150E 03      0.000E-01
                                   - 0.13 PAR   + .067 XO2N
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THE REACTIONS                                                                                      RATE CONSTANT  ACT. ENERGY(K)
 75     ROR   +    NO2          =                                                                  2.200E 04      0.000E-01
 76     ROR                     =  0.38 KET   + 0.38 HO2   + 0.62 AONE  + 0.62 D                   3.900E 05      0.000E-01
                                 - 1.24 PAR
 77     ROR                     =       ALD2  +      D     -      PAR                              9.000E 04      7.000E 03
 78     D     +    PAR          =       XO2   +      HO2   +  0.7 AONE  +  0.3 ALD2                1.000E 04      0.000E-01
                                 -  1.7 PAR
 79     D     +    KET          =       C2O3  -      PAR                                           1.000E 04      0.000E-01
 80     XO2   +    NO           =       NO2                                                        1.200E 04      0.000E-01
 81     KET                     =       C2O3  +      XO2   +      HO2   +       ALD2               3.000E-04      0.000E-01
                                 -    3 PAR
 82     O     +    OLE          =  0.95 ALD2  +  0.3 HO2   + 0.15 XO2   + 0.15 CO                  5.920E 03      3.240E 02
                                 + .05 MEO2   +  .05 C2O3  - 0.35 PAR
 83     OH    +    OLE          =       MEO2  +      ALD2  -      PAR                              4.200E 04     -5.370E 02
 84     O3    +    OLE          =   0.5 ALD2  +0.516 FORM  +  0.3 MCRG  +  0.3 CRIG                1.800E-02      1.897E 03
                                 +  .08 OH
 85     NO3   +    OLE          =  0.91 XO2   + 0.91 HO2   +  .09 XO2N                             1.140E 01      0.000E-01
 86     O     +    ETH          =       MEO2  +      HO2   +      CO                               1.080E 03      8.000E 02
 87     OH    +    ETH          =       MEO2  +      FORM                                          1.200E 04     -3.820E 02
 88     O3    +    ETH          =       FORM  + 0.37 CRIG  + 0.37 CO    + 0.13 HO2                 2.700E-03      2.840E 03

 89     CRIG  +    NO           =       FORM  +      NO2                                           1.000E 04      0.000E-01
 90     CRIG  +    NO2          =       FORM  +      NO3                                           1.000E 03      0.000E-01
 91     CRIG                    =                                                                  1.200E 02      0.000E-01
 92     CRIG  +    FORM         =                                                                  3.000E 01      0.000E-01
 93     CRIG  +    ALD2         =                                                                  3.000E 01      0.000E-01
 94     MCRG  +    NO           =       ALD2  +      NO2                                           1.000E 04      0.000E-01
 95     MCRG  +    NO2          =       ALD2  +      NO3                                           1.000E 03      0.000E-01
 96     MCRG                    =                                                                  1.200E 02      0.000E-01
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THE REACTIONS                                                                  RATE CONSTANT  ACT. ENERGY(K)
  97       MCRQ  +     FORM        =                                             3.000E 01      0.000E-01
  98       MCRQ  +     ALD2        =                                             3.000E 01      0.000E-01
  99       TOL   +     OH          =        HO2    + 0.64 XO2   + 1.13 GLY   + 0.56 MGLY     9.750E 03      0.000E-01
                                     + 0.36 PHEN   + 0.36 PAR   + .077 BZA
 100       PHEN  +     NO3         =        PHO    +      HNO3                              1.400E 04      0.000E-01
 101       BZA   +     OH          =        BZO2                                           2.000E 04      0.000E-01
 102       BZO2  +     NO2         =        PBZN                                           2.500E 03      0.000E-01
 103       BZO2  +     NO          =        XO2    +      PHO   +      CO    +      NO2    3.700E 03      0.000E-01
 104       PBZN                    =        BZO2   +      NO2                               2.200E-02      1.400E 04
 105       BZA                     =                                                       4.000E-03      0.000E-01
 106       PHO   +     NO2         =                                                       2.000E 04      0.000E-01
 107       XYL   +     OH          =        HO2    + 0.72 XO2   + 0.67 GLY   + 1.33 MGLY     3.600E 04      0.000E-01
                                     + 0.28 PHEN   + 0.56 PAR   +  .06 TLA
 108       TLA   +     OH          =        XO2    +      PHO   +    2 PAR                 2.000E 04      0.000E-01
 109       XO2   +     HO2         =                                                       1.000E 04      0.000E-01
 110       OH                      =        HO2                                            8.800E 01      0.000E-01
 111       NR                      =        NR                                             1.000E 00      0.000E-01
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                              THE FOLLOWING PHOTOLYSIS RATE CONSTANTS ARE USED

REACTION  SPECIES                                           ZENITH ANGLE (DEG)
   NO.                  0         10        20        30        40        50        60        70        78        86

    1      NO2      6.00E-01  5.95E-01  5.86E-01  5.64E-01  5.32E-01  4.85E-01  4.09E-01  2.88E-01  1.55E-01  3.49E-02
    8      O3       3.24E-03  3.14E-03  2.83E-03  2.31E-03  1.71E-03  1.08E-03  5.26E-04  1.59E-04  3.78E-05  4.53E-06
    9      O3       2.52E-02  2.50E-02  2.46E-02  2.37E-02  2.23E-02  2.04E-02  1.72E-02  1.21E-02  6.52E-03  1.47E-03
   21      HNO2     1.08E-01  1.07E-01  1.05E-01  1.02E-01  9.57E-02  8.73E-02  7.36E-02  5.19E-02  2.79E-02  6.28E-03
   26      H2O2     8.40E-04  8.33E-04  8.20E-04  7.90E-04  7.44E-04  6.79E-04  5.72E-04  4.03E-04  2.17E-04  4.89E-05
   30      NO3      1.84E 01  1.82E 01  1.79E 01  1.73E 01  1.63E 01  1.48E 01  1.25E 01  8.82E 00  4.75E 00  1.07E 00
   38      FORM     1.79E-03  1.77E-03  1.68E-03  1.54E-03  1.33E-03  1.07E-03  7.37E-04  3.96E-04  1.56E-04  2.65E-05
   39      FORM     2.39E-03  2.37E-03  2.30E-03  2.15E-03  1.95E-03  1.68E-03  1.30E-03  7.91E-04  3.77E-04  8.06E-05
   47      ALD2     4.29E-04  4.12E-04  3.93E-04  3.38E-04  2.79E-04  2.01E-04  1.24E-04  6.11E-05  1.86E-05  2.09E-06
   61      MNIT     1.80E-01  1.79E-01  1.76E-01  1.69E-01  1.60E-01  1.46E-01  1.23E-01  8.65E-02  4.66E-02  1.05E-02
   67      AONE     2.40E-05  2.38E-05  2.34E-05  2.26E-05  2.13E-05  1.94E-05  1.63E-05  1.15E-05  6.21E-06  1.40E-06
   69      GLY      4.50E-03  4.46E-03  4.39E-03  4.23E-03  3.99E-03  3.64E-03  3.07E-03  2.16E-03  1.16E-03  2.62E-04
   71      MGLY     1.20E-02  1.19E-02  1.17E-02  1.13E-02  1.06E-02  9.70E-03  8.17E-03  5.76E-03  3.10E-03  6.98E-04
   81      KET      1.80E-04  1.79E-04  1.76E-04  1.69E-04  1.60E-04  1.46E-04  1.23E-04  8.65E-05  4.66E-05  1.05E-05
  105      BZA      2.40E-03  2.38E-03  2.34E-03  2.26E-03  2.13E-03  1.94E-03  1.63E-03  1.15E-03  6.21E-04  1.40E-04
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EXAMPLE 5 - TEST RUN USING EKMA/CBM-X (STOICHIOMETRIC COEFF)


PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

       TEST CITY

LATITUDE     39.933

LONGITUDE    75.100

TIME ZONE    5.0

DATE         6      24     1980

TIME         800    TO     1800     LOCAL DAYLIGHT TIME


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS     INITIAL    250.      FINAL      1235.

TIMING                START      800.      STOP       1600.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME       800     900     1000    1100    1200    1300    1400    1500    1600

HEIGHT     250.0   413.6   619.2   811.8   954.3   1055.0  1129.0  1186.6  1235.0

REACTIVITY

EMISSIONS        ETH  FRACTION 0.040   OLE  FRACTION 0.030   ALD2 FRACTION 0.030

EMISSIONS        FORM FRACTION 0.020   TOL  FRACTION 0.120   XYL  FRACTION 0.100

EMISSIONS        PAR  FRACTION 0.510   NR   FRACTION 0.150

SURFACE LAYER    ETH  FRACTION 0.050   OLE  FRACTION 0.030   ALD2 FRACTION 0.160

SURFACE LAYER    FORM FRACTION 0.100   TOL  FRACTION 0.070   XYL  FRACTION 0.060

SURFACE LAYER    PAR  FRACTION 0.530   NR   FRACTION 0.000

ALOFT            ETH  FRACTION 0.060   OLE  FRACTION 0.030   ALD2 FRACTION 0.090

ALOFT            FORM FRACTION 0.060   TOL  FRACTION 0.080   XYL  FRACTION 0.070

ALOFT            PAR  FRACTION 0.610   NR   FRACTION 0.000

NO2/NOX      0.250
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TRANSPORTED CONCENTRATIONS

SURFACE LAYER        OZONE   0. 010      HYDROCARBON  0. 038   NOX      0. 000 PPM

ALOFT                OZONE   0. 070      HYDROCARBON  0. 040   NOX      0. 000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES     HOUR          1      2      3      4      5      6      7      8

  VOC     FRACTION     0. 170 0. 170 0. 170 0. 100 0. 020 0. 020 0. 020 0. 020

  NOX     FRACTION     0. 350 0. 350 0. 350 0. 190 0. 030 0. 030 0. 030 0. 070
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                              EXAMPLE 5 - TEST RUN USING EKMA/CBM-X (STOICHIOMETRIC COEFF)

  TIME      NMOC       NMOC/       NOX        NO2         O3         NO2         PAR
 (LDT )     TOTAL      NOX        TOTAL     FRACTION   (INSTANT)  (INSTANT)  (INSTANT)

  800.    1. 13800    9. 48333   0. 12000   0. 25000   0. 01000   0. 03000   0. 58114

  900.    0. 80001    8. 35948   0. 09570   0. 51914   0. 01747   0. 04968   0. 41330

 1000.    0. 59889    7. 83120   0. 07647   0. 66880   0. 03635   0. 05115   0. 31404

 1100.    0. 49405    7. 68795   0. 06426   0. 75163   0. 05595   0. 04830   0. 26332

 1200.    0. 42647    8. 36828   0. 05096   0. 80632   0. 08162   0. 04109   0. 23180

 1300.    0. 36260   10. 18771   0. 03559   0. 85215   0. 11343   0. 03033   0. 20177

 1400.    0. 30854   14. 23540   0. 02167   0. 88892   0. 14977   0. 01927   0. 17541

 1500.    0. 26035   23. 99836   0. 01085   0. 91693   0. 18620   0. 00995   0. 14975

 1600.    0. 22483   36. 24131   0. 00620   0. 93266   0. 21011   0. 00579   0. 12885

 1700.    0. 20533   49. 30787   0. 00416   0. 94353   0. 22755   0. 00393   0. 11654

 1800.    0. 19496   50. 64223   0. 00385   0. 95505   0. 23715   0. 00368   0. 10952

                    MAXIMUM O3    NOT REACHED. THE LAST ONE HOUR AVERAGE WAS 0. 23281 PPM.

                    MAXIMUM ONE HOUR AVE NO2   = 0. 05132 CENTERED AT  941.  LDT

                    MAXIMUM ONE HOUR AVE PAR   = 0. 49240 CENTERED AT  830.  LDT
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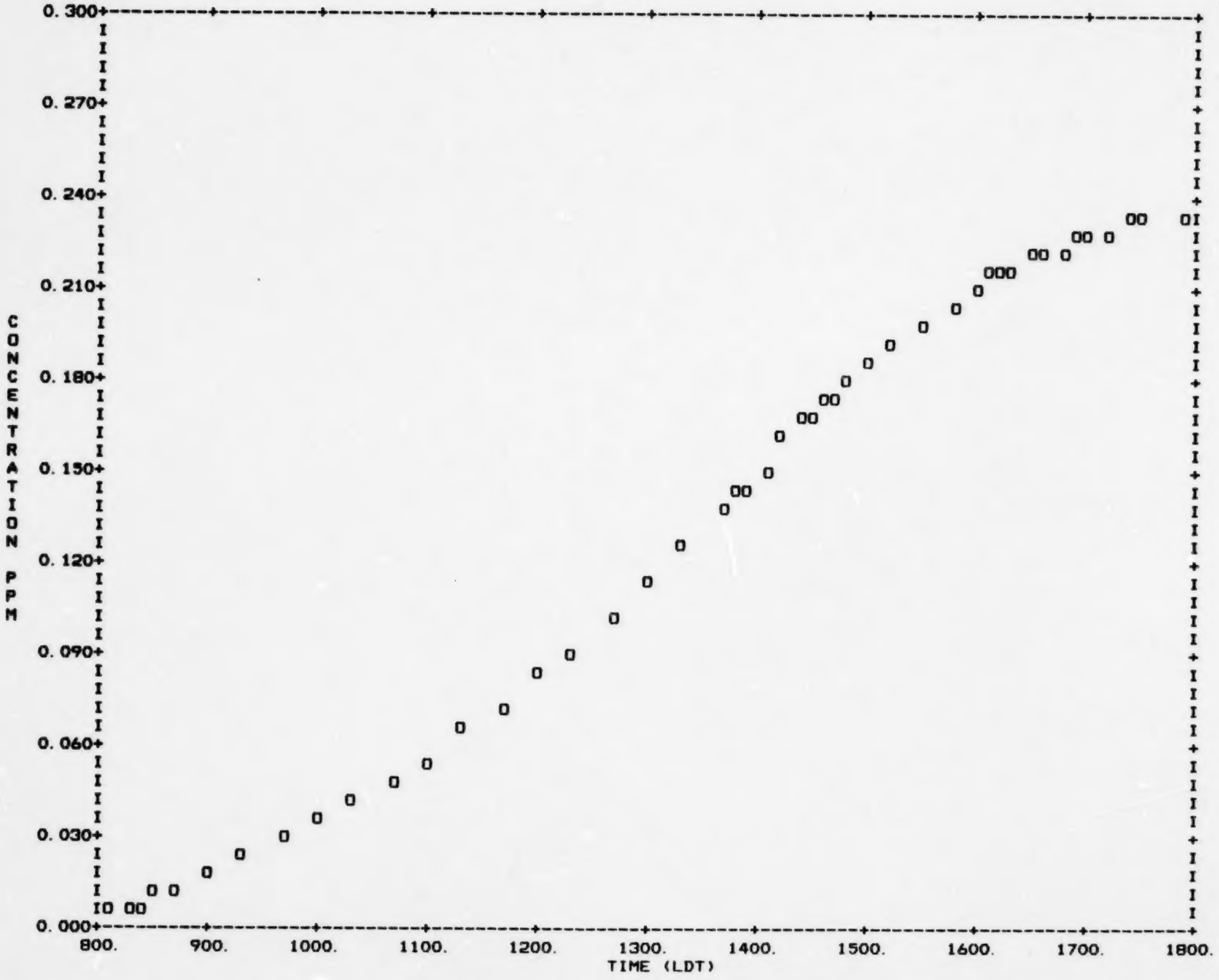
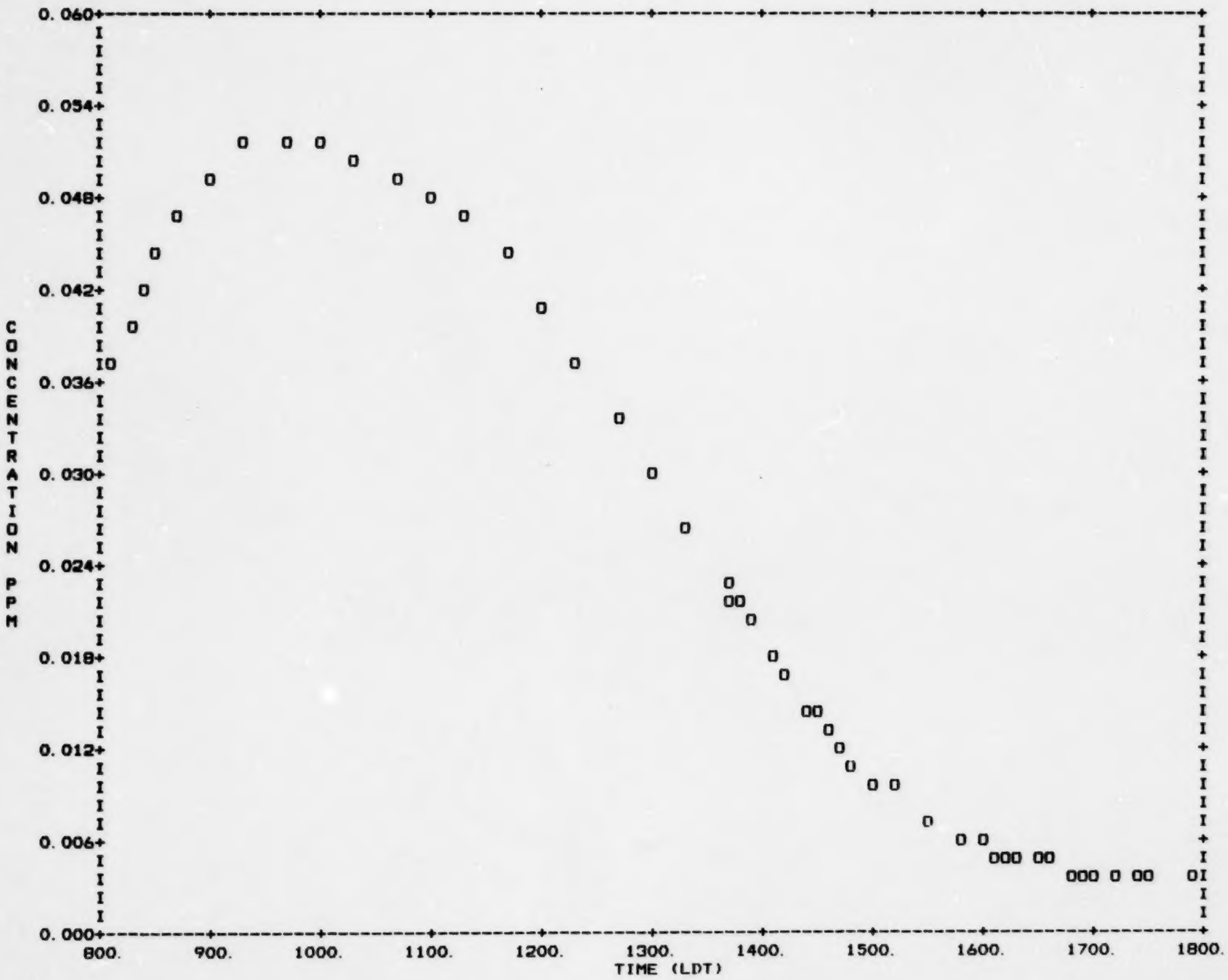


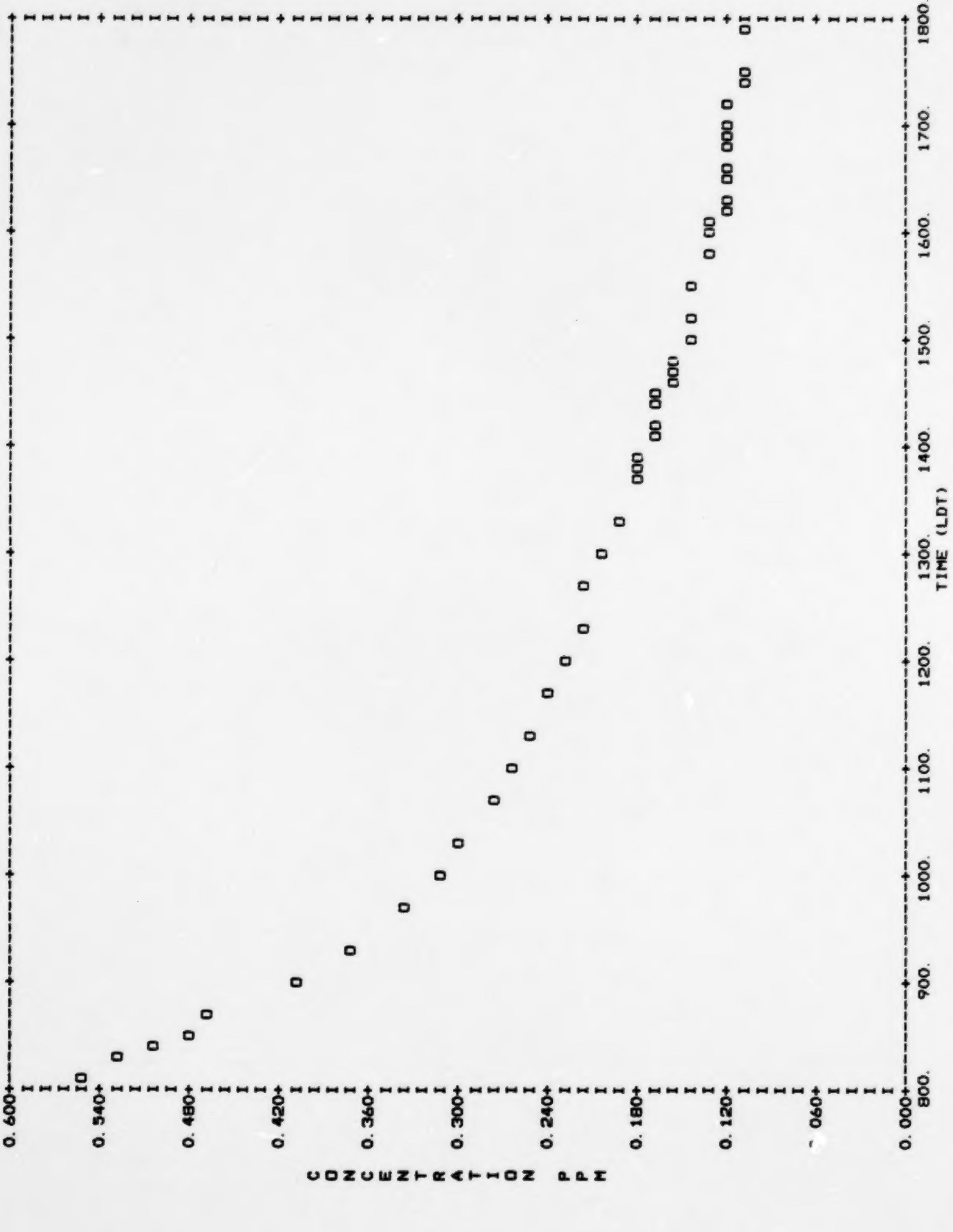
EXAMPLE 5 - TEST RUN USING EKMA/CBM-X (STOICHIOMETRIC COEFF)

O3 CONCENTRATION AS A FUNCTION OF TIME



EXAMPLE 5 - TEST RUN USING EKMA/CBM-X (STOICHIOMETRIC COEFF)

NO2 CONCENTRATION AS A FUNCTION OF TIME



EXAMPLE 5 - TEST RUN USING EKMA/CBM-X (STOICHIOMETRIC COEFF)

PAR CONCENTRATION AS A FUNCTION OF TIME

THE FOLLOWING PHOTOLYSIS RATE CONSTANTS ARE USED

REACTION NO.	SPECIES	ZENITH ANGLE (DEG) 0	10	20	30	40	50	60	70	78	86
1	NO2	6.00E-01	5.95E-01	5.86E-01	5.64E-01	5.32E-01	4.85E-01	4.09E-01	2.88E-01	1.55E-01	3.49E-02
8	O3	3.24E-03	3.14E-03	2.83E-03	2.31E-03	1.71E-03	1.08E-03	5.26E-04	1.59E-04	3.78E-05	4.53E-06
9	O3	2.52E-02	2.50E-02	2.46E-02	2.37E-02	2.23E-02	2.04E-02	1.72E-02	1.21E-02	6.52E-03	1.47E-03
21	HNO2	1.08E-01	1.07E-01	1.05E-01	1.02E-01	9.57E-02	8.73E-02	7.36E-02	5.19E-02	2.79E-02	6.28E-03
26	H2O2	8.40E-04	8.33E-04	8.20E-04	7.90E-04	7.44E-04	6.79E-04	5.72E-04	4.03E-04	2.17E-04	4.89E-05
30	NO3	1.84E 01	1.82E 01	1.79E 01	1.73E 01	1.63E 01	1.48E 01	1.25E 01	8.82E 00	4.75E 00	1.07E 00
38	FORM	1.79E-03	1.77E-03	1.68E-03	1.54E-03	1.33E-03	1.07E-03	7.37E-04	3.96E-04	1.56E-04	2.65E-05
39	FORM	2.39E-03	2.37E-03	2.30E-03	2.15E-03	1.95E-03	1.68E-03	1.30E-03	7.91E-04	3.77E-04	8.06E-05
47	ALD2	4.29E-04	4.12E-04	3.93E-04	3.38E-04	2.79E-04	2.01E-04	1.24E-04	6.11E-05	1.86E-05	2.09E-06
61	MNIT	1.80E-01	1.79E-01	1.76E-01	1.69E-01	1.60E-01	1.46E-01	1.23E-01	8.65E-02	4.66E-02	1.05E-02
67	AONE	2.40E-05	2.38E-05	2.34E-05	2.26E-05	2.13E-05	1.94E-05	1.63E-05	1.15E-05	6.21E-06	1.40E-06
69	GLY	4.50E-03	4.46E-03	4.39E-03	4.23E-03	3.99E-03	3.64E-03	3.07E-03	2.16E-03	1.16E-03	2.62E-04
71	MGLY	1.20E-02	1.19E-02	1.17E-02	1.13E-02	1.06E-02	9.70E-03	8.17E-03	5.76E-03	3.10E-03	6.98E-04
81	KET	1.80E-04	1.79E-04	1.76E-04	1.69E-04	1.60E-04	1.46E-04	1.23E-04	8.65E-05	4.66E-05	1.05E-05
105	BZA	2.40E-03	2.38E-03	2.34E-03	2.26E-03	2.13E-03	1.94E-03	1.63E-03	1.15E-03	6.21E-04	1.40E-04

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EXAMPLE 5 - TEST RUN USING EKMA/CBM-X (STOICHIOMETRIC COEFF)

PHOTOLYTIC RATE CONSTANTS CALCULATED FOR

        TEST CITY

LATITUDE     39.933

LONGITUDE    75.100

TIME ZONE    5.0

DATE         6     24    1980

TIME         800   TO    1800     LOCAL DAYLIGHT TIME

SOLAR NOON   1259

SUNRISE       538        SUNSET        2001


DILUTION DETERMINED FROM THE FOLLOWING

INVERSION HEIGHTS     INITIAL   250.      FINAL       1235.

TIMING                START     800.      STOP        1600.


MIXING HEIGHTS (AT THE BEGINNING OF EACH HOUR)

TIME       800      900      1000     1100     1200     1300     1400     1500     1600

HEIGHT     250.0    413.6    619.2    811.8    954.3    1055.0   1129.0   1186.6   1235.0


REACTIVITY

EMISSIONS        ETH  FRACTION 0.040   OLE  FRACTION 0.030   ALD2 FRACTION 0.030

EMISSIONS        FORM FRACTION 0.020   TOL  FRACTION 0.120   XYL  FRACTION 0.100

EMISSIONS        PAR  FRACTION 0.510   NR   FRACTION 0.150

SURFACE LAYER    ETH  FRACTION 0.050   OLE  FRACTION 0.030   ALD2 FRACTION 0.160

SURFACE LAYER    FORM FRACTION 0.100   TOL  FRACTION 0.070   XYL  FRACTION 0.060

SURFACE LAYER    PAR  FRACTION 0.530   NR   FRACTION 0.000

ALOFT            ETH  FRACTION 0.060   OLE  FRACTION 0.030   ALD2 FRACTION 0.090

ALOFT            FORM FRACTION 0.060   TOL  FRACTION 0.080   XYL  FRACTION 0.070

ALOFT            PAR  FRACTION 0.610   NR   FRACTION 0.000

NO2/NOX        0.250
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TRANSPORTED CONCENTRATIONS

SURFACE LAYER       OZONE   0.010     HYDROCARBON  0.038    NOX      0.000 PPM

ALOFT               OZONE   0.070     HYDROCARBON  0.040    NOX      0.000 PPM


CONTINUOUS EMISSIONS (EXPRESSED AS FRACTION OF THE INITIAL PRECURSORS)

SPECIES     HOUR          1     2     3     4     5     6     7     8

  VOC     FRACTION      0.170 0.170 0.170 0.100 0.020 0.020 0.020 0.020

  NOX     FRACTION      0.350 0.350 0.350 0.190 0.030 0.030 0.030 0.070
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THE FOLLOWING SIMULATIONS WERE DONE.

   NMOC      NOX       RATIO      O3         TIME      NO2         TIME      PAR        TIME
0. 00000  0. 00000   0. 00000  5. 2043E-02  1247.  0. 0000E-01  1730.  2. 2280E-02  1018.
0. 00000  0. 28000   0. 00000  1. 4744E-02  1438.  7. 3557E-02   830.  2. 3079E-02  1232.
2. 00000  0. 28000   7. 14286  1. 8555E-01  1800.  1. 0227E-01  1115.  8. 7880E-01   830.
2. 00000  0. 00000   0. 00000  4. 9269E-02  1219.  0. 0000E-01  1730.  8. 8222E-01   830.
1. 00000  0. 28000   3. 57143  4. 3796E-02  1719.  7. 8920E-02  1157.  4. 5077E-01   830.
2. 00000  0. 06314  31. 67642  2. 3221E-01  1800.  3. 5828E-02   850.  8. 7144E-01   830.
1. 47276  0. 20619   7. 14286  1. 8096E-01  1800.  7. 7188E-02  1050.  6. 5257E-01   830.
0. 98031  0. 13724   7. 14286  1. 8118E-01  1800.  5. 4036E-02   957.  4. 4136E-01   830.
0. 49016  0. 06862   7. 14286  1. 6512E-01  1800.  3. 0364E-02   917.  2. 3107E-01   830.
0. 44114  0. 06176   7. 14286  1. 5959E-01  1800.  2. 7781E-02   914.  2. 1003E-01   830.
1. 86605  0. 28000   6. 66446  1. 5937E-01  1800.  9. 9664E-02  1126.  8. 2148E-01   830.
1. 42748  0. 21419   6. 66446  1. 5778E-01  1800.  7. 8113E-02  1101.  6. 3333E-01   830.
0. 99594  0. 14944   6. 66446  1. 6006E-01  1800.  5. 7064E-02  1013.  4. 4816E-01   830.
0. 49797  0. 07472   6. 66446  1. 6339E-01  1800.  3. 2358E-02   920.  2. 3448E-01   830.
0. 44817  0. 06725   6. 66446  1. 5923E-01  1800.  2. 9651E-02   917.  2. 1311E-01   830.
1. 71067  0. 28000   6. 10954  1. 3140E-01  1800.  9. 6331E-02  1136.  7. 5517E-01   830.
1. 36854  0. 22400   6. 10954  1. 3248E-01  1800.  7. 8966E-02  1115.  6. 0824E-01   830.
0. 68427  0. 11200   6. 10954  1. 4657E-01  1800.  4. 4351E-02   940.  3. 1457E-01   830.
0. 34213  0. 05600   6. 10954  1. 4670E-01  1800.  2. 5270E-02   911.  1. 6765E-01   830.
0. 30792  0. 05040   6. 10954  1. 4253E-01  1800.  2. 3111E-02   908.  1. 5295E-01   830.
1. 57058  0. 28000   5. 60921  1. 0890E-01  1800.  9. 3137E-02  1144.  6. 9522E-01   830.
1. 25646  0. 22400   5. 60921  1. 1199E-01  1800.  7. 6720E-02  1122.  5. 6019E-01   830.
0. 62823  0. 11200   5. 60921  1. 2977E-01  1800.  4. 3749E-02   940.  2. 9054E-01   830.
0. 31412  0. 05600   5. 60921  1. 4238E-01  1800.  2. 5135E-02   911.  1. 5567E-01   830.
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0. 28270  0. 05040    5. 60921  1. 3898E-01    1800.  2. 3014E-02    908.  1. 4219E-01    830.
1. 44070  0. 28000    5. 14537  9. 0269E-02    1800.  9. 0072E-02   1151.  6. 3955E-01    830.
1. 15256  0. 22400    5. 14537  9. 4862E-02    1800.  7. 4551E-02   1125.  5. 1581E-01    830.
0. 57628  0. 11200    5. 14537  1. 1543E-01    1800.  4. 3234E-02    939.  2. 6832E-01    830.
0. 28814  0. 05600    5. 14537  1. 3790E-01    1800.  2. 5007E-02    911.  1. 4455E-01    830.
0. 25933  0. 05040    5. 14537  1. 3550E-01    1800.  2. 2908E-02    908.  1. 3218E-01    830.
1. 14125  0. 28000    4. 07588  5. 5310E-02    1800.  8. 2382E-02   1158.  5. 1133E-01    830.
0. 57062  0. 14000    4. 07588  7. 8578E-02    1800.  4. 9379E-02    952.  2. 6608E-01    830.
0. 56991  0. 13983    4. 07588  7. 8632E-02    1800.  4. 9336E-02    951.  2. 6577E-01    830.
0. 28496  0. 06991    4. 07588  1. 1382E-01    1800.  2. 9540E-02    918.  1. 4330E-01    830.
0. 25646  0. 06292    4. 07588  1. 2064E-01    1800.  2. 7183E-02    914.  1. 3105E-01    830.
2. 00000  0. 23510    8. 50698  2. 6117E-01    1800.  9. 2583E-02   1038.  8. 7813E-01    830.
1. 36046  0. 15992    8. 50698  2. 4059E-01    1800.  6. 4824E-02   1005.  6. 0402E-01    830.
0. 82715  0. 09723    8. 50698  2. 0365E-01    1800.  4. 1873E-02    930.  3. 7538E-01    830.
0. 41358  0. 04862    8. 50698  1. 5427E-01    1800.  2. 2943E-02    907.  1. 9804E-01    830.
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0. 37222  0. 04375    8. 50698  1. 4824E-01   1800.  2. 0894E-02   904.  1. 8029E-01   830.
2. 00000  0. 19020   10. 51513  3. 1832E-01   1800.  8. 1590E-02   957.  8. 7728E-01   830.
1. 30195  0. 12382   10. 51513  2. 5445E-01   1800.  5. 4587E-02   936.  5. 7836E-01   830.
0. 65098  0. 06191   10. 51513  1. 8142E-01   1800.  2. 9130E-02   912.  2. 9954E-01   830.
0. 32549  0. 03095   10. 51513  1. 3623E-01   1800.  1. 5475E-02   856.  1. 6004E-01   830.
0. 29294  0. 02786   10. 51513  1. 3101E-01   1800.  1. 4029E-02   855.  1. 4611E-01   830.
2. 00000  0. 14530   13. 76433  3. 0992E-01   1800.  6. 8801E-02   929.  8. 7587E-01   830.
1. 30965  0. 09515   13. 76433  2. 4479E-01   1800.  4. 5681E-02   918.  5. 8074E-01   830.
0. 65482  0. 04757   13. 76433  1. 7307E-01   1800.  2. 3690E-02   903.  3. 0071E-01   830.
0. 32741  0. 02379   13. 76433  1. 2959E-01   1800.  1. 2275E-02   851.  1. 6059E-01   830.
0. 29467  0. 02141   13. 76433  1. 2466E-01   1800.  1. 1093E-02   850.  1. 4656E-01   830.
2. 00000  0. 10040   19. 91949  2. 7775E-01   1800.  5. 2700E-02   907.  8. 7404E-01   830.
1. 34186  0. 06736   19. 91949  2. 2396E-01   1800.  3. 5287E-02   902.  5. 9318E-01   830.
0. 68997  0. 03464   19. 91949  1. 6225E-01   1800.  1. 8248E-02   853.  3. 1495E-01   830.
0. 34499  0. 01732   19. 91949  1. 2174E-01   1800.  9. 2079E-03   845.  1. 6761E-01   830.
0. 31049  0. 01559   19. 91949  1. 1713E-01   1800.  8. 2963E-03   844.  1. 5288E-01   830.
2. 00000  0. 05551   36. 03266  2. 1998E-01   1800.  3. 1893E-02   847.  8. 7057E-01   830.
1. 41464  0. 03926   36. 03266  1. 8660E-01   1800.  2. 2251E-02   845.  6. 2171E-01   830.
0. 77104  0. 02140   36. 03265  1. 4291E-01   1800.  1. 1889E-02   842.  3. 4798E-01   830.
0. 38552  0. 01070   36. 03265  1. 0865E-01   1800.  5. 8488E-03   837.  1. 8406E-01   830.
0. 34697  0. 00963   36. 03265  1. 0456E-01   1800.  5. 2547E-03   837.  1. 6768E-01   830.
1. 08275  0. 28000    3. 86696  5. 0290E-02   1800.  8. 0831E-02  1156.  4. 8617E-01   830.
2. 00000  0. 01120  178. 54370  1. 1646E-01   1800.  6. 3151E-03   831   8. 6928E-01   830
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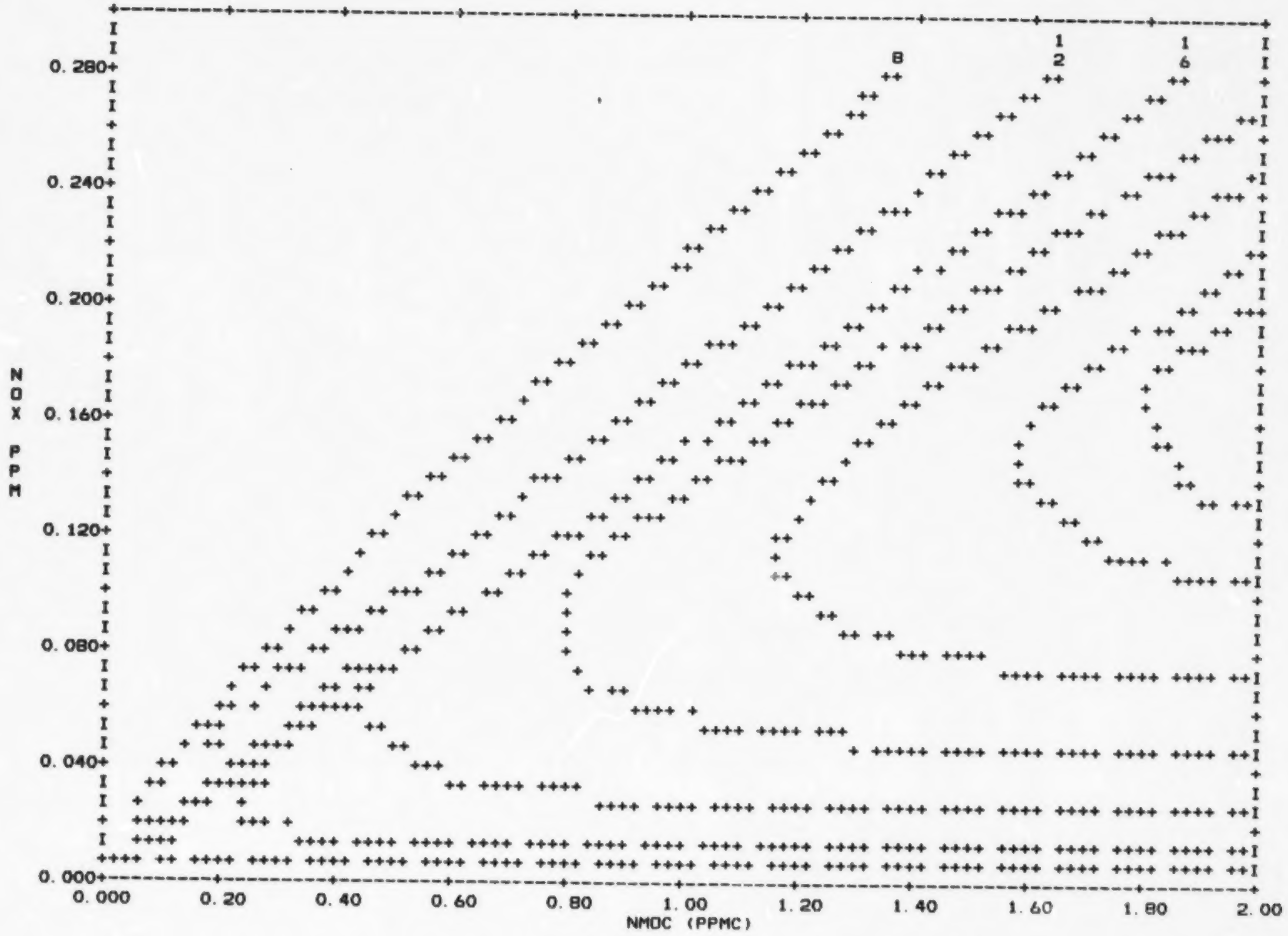

EXAMPLE 5 - TEST RUN USING EKMA/CBM-X (STOICHIOMETRIC COEFF)

THE O3 LINES ARE 0.08000 0.12000 0.16000 0.20000 0.24000 0.28000 0.30000

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Appendix A

THE EXPANDED CARBON-BOND MECHANISM (CBM-X)

TABLE A-1. The CBM-X mechanism as implemented in the computer code OZIPM-3.

1	NO2		= NO	+ O	1.000E+00	0.
2	O		= O3		4.440E+06	-6.900E+02
3	O3	+ NO	= NO2		2.660E+01	1.430E+03
4	O	+ NO2	= NO		1.380E+04	0.
5	O	+ NO2	= NO3		2.320E+03	-6.000E+02
6	O	+ NO	= NO2		3.120E+03	-4.110E+02
7	NO2	+ O3	= NO3		4.740E-02	2.450E+03
8	O3		= O1D		1.160E+00	0.
9	O3		= O		4.200E-02	0.
10	O1D		= O		4.290E+10	-1.000E+02
11	O1D		= OH	+ OH	6.520E+09	0.
12	O3	+ OH	= HO2		1.000E+02	9.400E+02
13	O3	+ HO2	= OH		3.000E+00	5.800E+02
14	NO3	+ NO	= NO2	+ NO2	2.810E+04	-2.500E+02
15	NO3	+ NO2	= NO	+ NO2	5.900E-01	1.230E+03
16	NO3	+ NO2	= N2O5		1.780E+03	6.000E+01
17	N2O5		= HNO3	+ HNO3	3.800E-02	0.
18	N2O5		= NO3	+ NO2	3.120E+00	1.084E+04
19	NO	+ NO2	= HNO2	+ HNO2	3.200E-07	0.
20	HNO2	+ HNO2	= NO	+ NO2	1.500E-05	0.
21	HNO2		= NO	+ OH	1.800E-01	0.
22	NO2	+ OH	= HNO3		1.630E+04	-5.600E+02
23	NO	+ OH	= HNO2		9.770E+03	-4.270E+02
24	HO2	+ NO	= OH	+ NO2	1.230E+04	-2.400E+02
25	NO	+ NO	= NO2	+ NO2	1.456E-04	-5.300E+02

TABLE A-1 (continued).

26	H2O2		= OH	+ OH		1.400E-03	0.
27	OH	+ H2O2	= HO2			2.520E+03	1.870E+02
28	OH	+ HNO2	= NO2			9.770E+03	0.
29	OH	+ HNO3	= NO3			1.920E+02	-7.780E+02
30	NO3		= NO2	+ O		2.600E+01	0.
31	NO3		= NO			4.600E+00	0.
32	HO2	+ HO2	= H2O2			4.144E+03	-1.150E+03
33	HO2	+ HO2	= H2O2			4.360E+03	-5.800E+03
34	HO2	+ NO2	= PNA			1.630E+03	-6.170E+02
35	PNA		= HO2	+ NO2		5.120E+00	1.042E+04
36	OH	+ CO	= HO2			4.000E+02	0.
37	FORM	+ HO2	= FROX			1.480E+01	0.
38	FORM	+ OH	= HO2	+ CO		1.500E+04	0.
39	FORM		= HO2	+ HO2	+ CO	1.100E+00	0.
40	FORM		= CO			1.060E+00	0.
41	FORM	+ O	= OH	+ HO2	+ CO	2.370E+02	1.550E+03
42	FORM	+ NO3	= HNO3	+ HO2	+ CO	9.300E-01	0.
43	FROX	+ NO	= FACD	+ NO2	+ HO2	1.040E+04	0.
44	FROX		= HO2	+ FORM		9.000E+01	0.
45	ALD2	+ O	= C2O3	+ OH		6.360E+02	9.860E+02
46	ALD2	+ OH	= C2O3			2.400E+04	-2.500E+02
47	ALD2	+ NO3	= C2O3	+ HNO3		3.700E+00	0.
48	ALD2		= MEO2	+ HO2	+ CO	1.110E+00	0.
49	ALD2	+ HO2	= MEO2	+ FORM		5.000E+00	0.
50	C2O3	+ NO	= MEO2	+ NO2		1.650E+04	-2.500E+02

TABLE A-1 (continued).

51	C2O3	+ NO2	= PAN				9.000E+03	-2.500E+02
52	PAN		= C2O3	+ NO2			2.220E-02	1.400E+04
53	MEO2	+ NO2	= MPNA				6.000E+03	-7.350E+02
54	MPNA		= MEO2	+ NO2			9.200E+01	1.040E+04
55	MEO2	+ NO	= MEO	+ NO2			1.100E+04	-1.800E+02
56	MEO	+ NO	= MNIT				4.440E+04	-2.000E+02
57	MEO	+ NO	= FORM	+ HO2	+ NO		1.920E+03	0.
58	MEO	+ NO2	= MEN3				2.220E+04	0.
59	MEO		= FORM	+ HO2			3.760E+05	1.313E+03
60	MEN3	+ OH	= FORM	+ NO2			2.220E+03	3.600E+02
61	MNIT	+ OH	= FORM	+ NO			2.370E+03	3.400E+02
62	MNIT		= MEO	+ NO			3.000E-01	0.
63	MEO2	+ MEO2	= MEO	+ MEO			1.750E+02	-2.200E+02
64	MEO2	+ MEO2	= FORM	+ MEOH			3.280E+02	-2.200E+02
65	MEO2	+ C2O3	= MEO	+ MEO2			4.400E+03	0.
66	C2O3	+ C2O3	= MEO2	+ MEO2			3.700E+03	0.
67	MEO2	+ HO2	= PROX				8.900E+03	-1.300E+03
68	C2O3	+ HO2	= PROX				9.600E+03	0.
69	AONE		= MEO2	+ C2O3			4.000E-05	0.
70	AONE	+ OH	= ANO2				5.800E+02	0.
71	ANO2	+ NO	= NO2	+ FORM	+ C2O3		1.200E+04	0.
72	GLY		= CO	+ CO			5.200E-03	0.
73	GLY		= CO	+ FORM			1.600E-03	0.
74	GLY		= HO2	+ HO2	+ CO	+ CO	7.000E-04	0.
75	GLY	+ OH	= HO2	+ CO	+ CO		1.500E+04	0.

TABLE A-1 (continued).

76	MGLY		= C2O3	+ HO2	+ CO		2.000E-02	0.
77	MGLY	+ OH	= MGPX				2.600E+04	0.
78	MGPX	+ NO	= C2O3	+ NO2			1.200E+04	0.
79	OH		= MEO2				2.100E+01	0.
80	PAR	+ OH	= RO2				1.500E+02	0.
81	PAR	+ OH	= RO2R				1.000E+03	0.
82	RO2	+ NO	= NO2	+ HO2	+ ALD2	+ X	1.200E+04	0.
83	RO2R	+ NO	= NO2	+ ROR			1.200E+04	0.
84	RO2R	+ NO	= NTR				1.000E+03	0.
85	ROR	+ NO2	= NTR				2.200E+04	0.
86	ROR		= KET	+ HO2			1.500E+05	0.
87	ROR		= ALD2	+ D	+ X		9.000E+04	7.000E+03
88	ROR		= AONE	+ D	+ X	+ X	2.400E+05	0.
89	X	+ PAR	=				1.000E+04	0.
90	D	+ PAR	= RO2				3.000E+03	0.
91	D	+ PAR	= AO2	+ X	+ X		7.000E+03	0.
92	D	+ KET	= C2O3	+ X			1.000E+04	0.
93	AO2	+ NO	= NO2	+ HO2	+ AONE		1.200E+04	0.
94	KET		= C2O3	+ RO2	+ X	+ X	3.000E-04	0.
95	O	+ OLE	= MEO2	+ C2O3	+ X		3.000E+02	3.240E+02
96	O	+ OLE	= RO2	+ HO2	+ CO	+ X	8.800E+02	3.240E+02
97	O	+ OLE	= ALD2				4.740E+03	3.240E+02
98	OH	+ OLE	= MEO2	+ ALD2	+ X		4.200E+04	-5.370E+02
99	O3	+ OLE	= ALD2	+ CRIG	+ X		5.400E-03	1.897E+03
100	O3	+ OLE	= FORM	+ MCRG	+ X		5.400E-03	1.897E+03

TABLE A-1 (continued).

101	O3	+ OLE	= ALD2	+ HOTA	+ X		3.600E-03	1.897E+03
102	O3	+ OLE	= FORM	+ HTMA	+ X		3.600E-03	1.897E+03
103	NO3	+ OLE	= PNO2				1.140E+01	0.
104	O	+ ETH	= MEO2	+ HO2	+ CO		1.080E+03	8.000E+02
105	OH	+ ETH	= MEO2	+ FORM			1.200E+04	-3.820E+02
106	O3	+ ETH	= FORM	+ CRIG			1.000E-03	2.840E+03
107	O3	+ ETH	= FORM	+ HOTA			1.700E-03	2.840E+03
108	HOTA		=				2.500E+01	0
109	HOTA		= CO				5.800E+01	0.
110	HOTA		= HO2	+ HO2			1.000E+01	0.
111	HOTA		= FACD				7.000E+00	0.
112	HTMA		=				2.000E+02	0.
113	HTMA		= MEO2	+ CO	+ OH		4.000E+02	0.
114	HTMA		= MEO2	+ HO2			3.200E+02	0.
115	HTMA		= HO2	+ CO	+ FORM	+ HO2	8.000E+01	0.
116	CRIG	+ NO	= FORM	+ NO2			1.000E+04	0.
117	CRIG	+ NO2	= FORM	+ NO3			1.000E+03	0.
118	CRIG	+ H2O	= FACD				6.000E-03	0.
119	CRIG	+ FORM	= OZD				3.000E+01	0.
120	CRIG	+ ALD2	= OZD				3.000E+01	0
121	MCRG	+ NO	= ALD2	+ NO2			1 000E+04	0
122	MCRG	+ NO2	= ALD2	+ NO3			1.000E+03	0.
123	MCRG	+ H2O	= ACAC				6.000E-03	0.
124	MCRG	+ FORM	= OZD				3.000E+01	0.
125	MCRG	+ ALD2	= OZD				3.000E+01	0.

TABLE A-1 (concluded).

126	PNO2	+ NO	= DNIT				1. 000E+03	0.
127	PNO2	+ NO	= NTR	+ HO2	+ NO2		1. 000E+04	0.
128	TOL	+ OH	= OPEN	+ GLY			5. 500E+03	0.
129	TOL	+ OH	= PHEN	+ HO2	+ PAR		3. 500E+03	0.
130	TOL	+ OH	= BO2				7. 500E+02	0.
131	OPEN	+ NO	= NO2	+ HO2	+ MGLY	+ GLY	1. 000E+04	0.
132	PHEN	+ NO3	= PHO	+ HNO3			1. 400E+04	0.
133	BZA	+ OH	= BZO2				2. 000E+04	0.
134	BZO2	+ NO2	= PBZN				2. 500E+03	0.
135	BZO2	+ NO	= NO2	+ PHO2	+ CO		3. 700E+03	0.
136	BO2	+ NO	= NO2	+ BZA	+ HO2		1. 200E+04	0.
137	PBZN		= BZO2	+ NO2			2. 200E-02	1. 400E+04
138	BZA		= PROD				4. 000E-03	0.
139	PHO	+ NO2	= NPHN				2. 000E+04	0.
140	PHO2	+ NO	= NO2	+ PHO			1. 200E+04	0.
141	XYL	+ OH	= XYLO				2. 000E+03	0.
142	XYLO	+ NO	= NO2	+ HO2	+ TLA		1. 200E+04	0.
143	TLA	+ OH	= TLO2				2. 000E+04	0.
144	TLO2	+ NO	= NO2	+ PHO	+ PAR	+ PAR	4. 000E+03	0.
145	XYL	+ OH	= HO2	+ PHEN	+ PAR	+ PAR	1. 000E+04	0.
146	XYL	+ OH	= OPEN	+ MGLY			2. 400E+04	0.
147	OH		= HO2				8. 800E+01	0.
148	NR		= NR				1. 000E+00	0.

APPENDIX B

CBM-X CARBON BOND GROUPS FOR ORGANIC SPECIES

Table B-1. Molecular weights of molecules (in alphabetical order).

SAROAD Code	Chemical Name	Molecular Weight
43814	1,1,1-TRICHLOROETHANE	133.42
43820	1,1,2-TRICHLOROETHANE	131.66
43813	1,1-DICHLOROETHANE	98.97
99013	1,1-DICHLOROETHENE	96.95
45225	1,2,3-TRIMETHYLBENZENE	120.19
45208	1,2,4-TRIMETHYLBENZENE	120.19
99016	1,2-DICHLOROPROPANE	112.99
45207	1,3,5-TRIMETHYLBENZENE	120.19
43218	1,3-BUTADIENE	54.09
46201	1,4-DIOXANE	88.12
98104	1-CHLOROBUTANE	92.57
43268	1-DECENE	140.27
98111	1-ETHOXY-2-PROPANOL	104.15
98113	1-HEPTANOL	116.21
98005	1-HEPTENE	98.18
43245	1-HEXENE	84.16
98037	1-METHYLCYCLOHEXANE	96.17
43267	1-NONENE	127.05
43224	1-PENTENE	70.13
43312	1-T-2-C-4-TM-CYCLOPENTANE	112.23
43269	1-UNDECENE	154.30
43296	2,2,3-TRIMETHYLPENTANE	114.23
43276	2,2,4-TRIMETHYLPENTANE	114.22
98033	2,2,5-TRIMETHYLHEXANE	128.26
43299	2,2,5-TRIMETHYLPENTANE	114.23
43291	2,2-DIMETHYLBUTANE	86.17
43280	2,3,3-TRIMETHYLPENTANE	114.22
43279	2,3,4-TRIMETHYLPENTANE	114.22
43234	2,3-DIMETHYL-1-BUTENE	84.16
98001	2,3-DIMETHYLBUTANE	86.17
43274	2,3-DIMETHYLPENTANE	100.20
98054	2,4,4-TRIMETHYL-1-PENTENE	112.22
98055	2,4,4-TRIMETHYL-2-PENTENE	112.22
43277	2,4-DIMETHYLHEXANE	114.22
43271	2,4-DIMETHYLPENTANE	100.20
43278	2,5-DIMETHYLHEXANE	114.22
98110	2-(2-BUTOXYETHOXY)-ETHANOL	162.18
43308	2-BUTYLETHANOL	118.17
98108	2-BUTYLTETRAHYDROFURAN	128.19
98051	2-CHLOROTOLUENE	126.59
43311	2-ETHOXYETHANOL	90.12
43452	2-ETHOXYETHYL ACETATE	132.00
98002	2-ETHYL-1-BUTENE	84.16
98112	2-ETHYL-1-HEXANOL	130.23

Table B-1. (continued)

SAROAD Code	Chemical Name	Molecular Weight
43310	2-METHOXYETHANOL	76.09
43229	2-METHYL PENTANE	86.17
43225	2-METHYL-1-BUTENE	70.13
98040	2-METHYL-1-PENTENE	84.16
43228	2-METHYL-2-BUTENE	70.13
98004	2-METHYL-2-PENTENE	84.16
98076	2-METHYL-3-HEXANONE	114.19
43275	2-METHYLHEXANE	100.20
98032	3,5,5-TRIMETHYLHEXANE	128.26
98105	3-(CHLOROMETHYL)-HEPTANE	148.68
99021	3-CARENE	136.23
98041	3-HEPTENE	98.19
43230	3-METHYL PENTANE	86.17
43223	3-METHYL-1-BUTENE	70.13
43211	3-METHYL-1-PENTENE	84.16
43270	3-METHYL-T-2-PENTENE	84.16
43298	3-METHYLHEPTANE	114.23
43295	3-METHYLHEXANE	100.20
43293	4-METHYL-T-2-PENTENE	84.16
43297	4-METHYLHEPTANE	114.23
98042	4-NONENE	127.05
45221	A-METHYLSTYRENE	118.15
98025	A-PINENE	136.24
98097	A-TERPINEOL	154.24
43503	ACETALEHYDE	44.05
43404	ACETIC ACID	60.05
43551	ACETONE	58.08
43702	ACETONITRILE	41.05
43206	ACETYLENE	26.04
43505	ACROLEIN (ACRYLIC ALDHYDE)	56.06
43704	ACRYLONITRILE	53.06
98078	ALKENE KETONE	72.10
98085	ALKYL SUSTITUTED CYCLOHEXANE	132.21
99001	ALLYL CHLORIDE	76.53
98015	ANTHRACENE	178.22
98020	B-METHYLSTYRENE	118.15
98026	B-PINENE	136.24
45201	BENZENE	78.11
45402	BENZOIC ACID	122.13
98024	BENZYL CHLORIDE	126.56
99017	BROMODICHLOROMETHANE	163.82
99019	BROMOFORM	252.77

Table B-1. (continued)

SAROAD Code	Chemical Name	Molecular Weight
98080	BUTANDIOL	90.12
43213	BUTENE	56.10
98074	BUTYL CELLOSOLVE	118.17
43510	BUTYRALDEHYDE	72.12
98035	C-2-HEXENE	84.16
43266	C-2-OCTENE	112.22
98003	C-3-HEXENE	84.16
43115	C-7 CYCLOPARAFFINS	98.19
43116	C-8 CYCLOPARAFFINS	112.23
43117	C-9 CYCLOPARAFFINS	126.26
98050	C10 AROMATICS	134.22
98039	C10 OLEFINS	140.27
98086	C2 ALKYL DECALIN	166.27
98084	C2 ALKYL INDAN	146.23
98064	C2 CYCLOHEXANE	112.22
43511	C3 ALDEHYDE	58.08
98068	C3 ALKYL CYCLOHEXANE	126.24
98065	C3 CYCLOHEXANE	126.24
98069	C4 ALKYL CYCLOHEXANE	140.27
98066	C4 CYCLOHEXANE	140.27
98070	C4 SUBSTITUTED CYCLOHEXANE	142.28
98073	C4 SUBSTITUTED CYCLOHEXANONE	154.26
43512	C5 ALDEHYDE	86.14
98067	C5 CYCLOHEXANE	154.30
98075	C5 ESTER	130.19
98071	C5 SUBSTITUTED CYCLOHEXANE	154.30
98095	C6 ALDEHYDE	100.17
43289	C6 OLEFINS	84.16
98072	C6 SUBSTITUTED CYCLOHEXANE	170.32
98093	C7 ESTER	158.24
43294	C7-OLEFINS	98.18
43513	C8 ALDEHYDE	128.21
43290	C8 OLEFINS	112.23
98049	C9 AROMATICS	120.20
98038	C9 OLEFINS	127.05
98096	CARBITOL	134.17
98030	CARBON SULFIDE	76.14
43807	CARBON TETRABROMIDE	331.67
43804	CARBON TETRACHLORIDE	153.84
98031	CARBONYL SULFIDE	60.08
98087	CARVOMENTHOL	156.27
98088	CARVONE	150.22
43443	CELLOSOLVE ACETATE	132.00

Table B-1. (continued)

SAROAD Code	Chemical Name	Molecular Weight
99020	CHLORODIBROMOMETHANE	208.27
43825	CHLORODIFLUOROMETHANE (F-22)	86.47
43830	CHLOROFLUOROHYDROCARBONS	118.00
43803	CHLOROFORM	119.39
43827	CHLOROPENTAFLUOROETHANE(F-115)	154.47
99003	CHLOROPRENE	88.54
43826	CHLOROTRIFLUOROMETHANE (F-13)	104.46
43217	CIS-2-BUTENE	56.10
43227	CIS-2-PENTENE	70.13
98019	CRYOFLOURANE (F 114)	170.93
43248	CYCLOHEXANE	84.16
43264	CYCLOHEXANONE	98.15
43273	CYCLOHEXENE	82.14
43242	CYCLOPENTANE	70.14
43292	CYCLOPENTENE	68.11
43207	CYCLOPROPANE	42.08
98027	D-LIMONENE	136.24
43320	DIACETONE ALCOHOL	116.16
99015	DIBENZOFURAN	168.18
98107	DIBUTYL ETHER	130.23
43823	DICHLORODIFLOUROMETHANE (F-12)	120.91
43802	DICHLOROMETHANE	84.94
43828	DICHLOROTETRAFLUOROETHANE/114	170.92
98062	DIETHYLCYCLOHEXANE	140.27
98018	DIMETHYL ETHER	46.07
43450	DIMETHYL FORMAMIDE	73.09
98059	DIMETHYLCYCLOHEXANE	112.12
45103	DIMETHYLETHYLBENZENE	134.21
98091	DIMETHYLHEPTANE	128.26
98012	DIMETHYLNAPHTHALENE	156.22
98017	DM-2,3,DH-1H-INDENE	146.23
43287	DOCOSANE	310.59
43285	EICOSANE	282.54
99006	EPICHLOROHYDRIN	92.53
43202	ETHANE	30.07
43433	ETHYL ACETATE	88.10
43438	ETHYL ACRYLATE	100.11
43302	ETHYL ALCOHOL	46.07
43812	ETHYL CHLORIDE	64.52
43351	ETHYL ETHER	74.12
98106	ETHYL ISOPROPYL ETHER	88.15
43219	ETHYLACETYLENE	54.09
43721	ETHYLAMINE	45.09

Table B-1. (continued)

SAROAD Code	Chemical Name	Molecular Weight
45203	ETHYLBENZENE	106.16
43288	ETHYLCYCLOHEXANE	112.23
98061	ETHYLCYCLOHEXANE	112.22
98057	ETHYLCYCLOPENTANE	98.19
43203	ETHYLENE	28.05
99014	ETHYLENE DIBROMIDE	187.88
43815	ETHYLENE DICHLORIDE	99.00
43370	ETHYLENE GLYCOL	62.07
43601	ETHYLENE OXIDE	44.05
98082	ETHYLHEPTENE	127.05
98011	ETHYLNAPHTHALENE	156.22
43502	FORMALDEHYDE	30.03
43368	GLYCOL	62.07
43367	GLYCOL ETHER	62.07
43286	HENEICOSANE	296.57
43282	HEPTADECANE	240.46
43232	HEPTANE	100.20
98077	HEPTANONE	114.18
99007	HEXACHLOROCYCLOPENTADIENE	272.77
43281	HEXADECANE	226.44
43231	HEXANE	86.17
43371	HEXYLENE GLYCOL	118.18
98044	INDAN	118.18
98048	INDENE	116.16
98115	ISOAMYL ISOBUTYRATE	158.24
43214	ISOBUTANE	58.12
43446	ISOBUTYL ACETATE	116.16
43306	ISOBUTYL ALCOHOL	74.12
43451	ISOBUTYL ISOBUTYRATE	144.21
98047	ISOBUTYLBENZENE	134.22
43215	ISOBUTYLENE	56.10
98036	ISOBUTYRALDEHYDE	72.11
43120	ISOMERS OF BUTENE	56.10
45105	ISOMERS OF BUTYLBENZENE	134.21
43109	ISOMERS OF DECANE	142.28
45106	ISOMERS OF DIETHYLBENZENE	134.21
43112	ISOMERS OF DODECANE	170.33
45104	ISOMERS OF ETHYLTOLUENE	120.19
43106	ISOMERS OF HEPTANE	100.20
43105	ISOMERS OF HEXANE	86.17
43108	ISOMERS OF NONANE	128.25
43107	ISOMERS OF OCTANE	114.23
43114	ISOMERS OF PENTADECANE	212.41

Table B-1. (continued)

SAROAD Code	Chemical Name	Molecular Weight
43122	ISOMERS OF PENTANE	72.15
43121	ISOMERS OF PENTENE	70.13
43113	ISOMERS OF TETRADECANE	198.38
43111	ISOMERS OF TRIDECANE	184.36
43110	ISOMERS OF UNDECANE	156.30
45102	ISOMERS OF XYLENE	106.16
43243	ISOPRENE	68.13
43444	ISOPROPYL ACETATE	104.00
43304	ISOPROPYL ALCOHOL	60.09
98043	ISOPROPYLBENZENE (CUMENE)	120.20
98089	ISOPULEGONE	154.26
98056	ISOVALERALDEHYDE	86.14
43119	LACTOL SPIRITS	114.23
98022	M-CRESOL (3-M-BENZENOL)	110.16
98045	M-DIETHYLBENZENE	134.22
45212	M-ETHYLTOLUENE	120.19
45205	M-XYLENE	106.16
99008	MALEIC ANHYDRIDE	98.06
43201	METHANE	16.04
43432	METHYL ACETATE	74.08
43301	METHYL ALCOHOL	32.04
43445	METHYL AMYL ACETATE	140.00
43561	METHYL AMYL KETONE	114.19
43819	METHYL BROMIDE	94.95
43801	METHYL CHLORIDE	50.49
43552	METHYL ETHYL KETONE	72.10
98090	METHYL HEPTENE	112.22
43560	METHYL ISOBUTYL KETONE	100.16
98114	METHYL ISOBUTYRATE	102.13
43559	METHYL N-BUTYL KETONE	100.16
43209	METHYLACETYLENE	40.06
98016	METHYLANTHRACENE	192.25
43261	METHYLCYCLOHEXANE	85.16
43262	METHYLCYCLOPENTANE	84.16
43272	METHYLCYCLOPENTENE	82.14
43805	METHYLENE BROMIDE	173.85
98010	METHYLNAPHTHALENE	142.19
45234	METHYLPROPYLBENZENE	134.21
43118	MINERAL SPIRITS	114.23
45801	MONOCHLOROBENZENE	112.56
43212	N-BUTANE	58.12
43435	N-BUTYL ACETATE	116.16
43305	N-BUTYL ALCOHOL	74.12

Table B-1. (continued)

SAROAD Code	Chemical Name	Molecular Weight
43238	N-DECANE	142.28
43255	N-DODECANE	170.33
43260	N-PENTADECANE	212.41
43220	N-PENTANE	72.15
98063	N-PENTYLCYCLOHEXANE	154.30
43303	N-PROPYL ALCOHOL	60.09
45209	N-PROPYLBENZENE	120.19
43259	N-TETRADECANE	198.38
43258	N-TRIDECANE	184.36
45101	NAPHTHA	114.23
98046	NAPHTHALENE	128.19
99009	NITROBENZENE	123.11
99010	NITROSOMORPHOLINE	116.11
43284	NONADECANE	268.51
43235	NONANE	128.25
98021	O-CRESOL (2-M-BENZENOL)	110.16
45211	O-ETHYLTOLUENE	120.19
45204	O-XYLENE	106.16
43283	OCTADECANE	254.49
43233	OCTANE	114.23
43265	OCTENE	112.21
98023	P-CRESOL (4-M-BENZENOL)	110.16
45807	P-DICHLOROBENZENE	147.01
45206	P-XYLENE	106.16
98094	PENTYL ALCOHOL	88.15
43817	PERCHLOROETHYLENE	165.85
45300	PHENOLS	94.11
43850	PHOSGENE (CCL2O)	98.92
98028	PHTHALIC ANAHYDRIDE	148.00
43208	PROPADIENE	40.06
43204	PROPANE	44.09
43504	PROPRIONALDEHYDE	58.08
43434	PROPYL ACETATE	102.13
45108	PROPYLBENZENE	120.19
98109	PROPYLCYCLOHEXANONE	140.23
43205	PROPYLENE	42.08
43369	PROPYLENE GLYCOL	76.09
43602	PROPYLENE OXIDE	58.08
98013	PROPYLNAPHTHALENE	170.25
45216	SEC-BUTYLBENZENE	134.21
45220	STYRENE	104.14
98116	SUBSTITUTED C7 ESTER (C12)	211.19
98117	SUBSTITUTED C9 ESTER (C12)	218.24

Table B-1. (concluded)

SAROAD Code	Chemical Name	Molecular Weight
98034	T-2-HEXENE	84.16
98052	T-BUTYLBENZENE	134.22
43123	TERPENES	136.24
98079	TERPINENE	136.23
43309	TERT-BUTYL ALCOHOL	74.12
45215	TERT-BUTYLBENZENE	134.21
43390	TETRAHYDROFURAN	72.10
45232	TETRAMETHYLBENZENE	134.21
45202	TOLUENE	92.13
99018	TRANS-1,2-DICHLOROETHENE	96.95
43216	TRANS-2-BUTENE	56.10
43226	TRANS-2-PENTENE	70.13
45233	TRI/TETRAALKYL BENZENE	148.23
43824	TRICHLOROETHYLENE	131.40
43811	TRICHLOROFLOUROMETHANE	137.38
43821	TRICHLOROTRIFLOUROETHANE	187.38
43740	TRIMETHYL AMINE	59.11
45107	TRIMETHYLBENZENE	120.19
98060	TRIMETHYLCYCLOHEXANE	129.27
98058	TRIMETHYLCYCLOPENTANE	112.16
98083	TRIMETHYLDECENE	182.35
43822	TRIMETHYLFLUOROSILANE	92.00
98014	TRIMETHYLNAPHTHALENE	170.25
43241	UNDECANE	156.30
43860	VINYL CHLORIDE	62.50
45401	XYLENE BASE ACIDS	230.00

TABLE B-2. Species profiles by bond groups for CBM-X.

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
43814	1,1,1-TRICHLOROETHANE	--	--	--	--	--	--	--	2
43820	1,1,2-TRICHLOROETHANE	--	--	--	--	--	--	--	2
43813	1,1-DICHLOROETHANE	--	--	--	--	--	--	--	2
99013	1,1-DICHLOROETHENE	--	--	--	--	--	--	1	--
45225	1,2,3-TRIMETHYLBENZENE	--	1	--	1	--	--	--	--
45208	1,2,4-TRIMETHYLBENZENE	--	1	--	1	--	--	--	--
99016	1,2-DICHLOROPROPANE	--	2	--	--	--	--	--	1
45207	1,3,5-TRIMETHYLBENZENE	--	1	--	1	--	--	--	--
43218	1,3-BUTADIENE	1	--	--	--	2	--	--	--
46201	1,4-DIOXANE	1	--	--	--	--	1	--	--
98104	1-CHLOROBUTANE	--	4	--	--	--	--	--	--
43268	1-DECENE	1	8	--	--	--	--	--	--
98111	1-ETHOXY-2-PROPANOL	--	4	--	--	1	--	--	--
98113	1-HEPTANOL	--	6	--	--	1	--	--	--
98005	1-HEPTENE	1	5	--	--	--	--	--	--
43245	1-HEXENE	1	4	--	--	--	--	--	--
98037	1-METHYLCYCLOHEXANE	--	7	--	--	--	--	--	--
43267	1-NONENE	1	7	--	--	--	--	--	--
43224	1-PENTENE	1	3	--	--	--	--	--	--
43312	1-T-2-C-4-TM-CYCLOPENTANE	--	8	--	--	--	--	--	--
43269	1-UNDECENE	1	9	--	--	--	--	--	--
43296	2,2,3-TRIMETHYLPENTANE	--	8	--	--	--	--	--	--
43276	2,2,4-TRIMETHYLPENTANE	--	8	--	--	--	--	--	--
98033	2,2,5-TRIMETHYLHEXANE	--	9	--	--	--	--	--	--
43299	2,2,5-TRIMETHYLPENTANE	--	8	--	--	--	--	--	--
43291	2,2-DIMETHYLBUTANE	--	6	--	--	--	--	--	--

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
43280	2,3,3-TRIMETHYLPENTANE	--	8	--	--	--	--	--	--
43279	2,3,4-TRIMETHYLPENTANE	--	8	--	--	--	--	--	--
43234	2,3-DIMETHYL-1-BUTENE	1	4	--	--	--	--	--	--
98001	2,3-DIMETHYLBUTANE	--	6	--	--	--	--	--	--
43274	2,3-DIMETHYLPENTANE	--	7	--	--	--	--	--	--
98054	2,4,4-TRIMETHYL-1-PENTENE	1	6	--	--	--	--	--	--
98055	2,4,4-TRIMETHYL-2-PENTENE	--	4	--	--	--	2	--	--
43277	2,4-DIMETHYLHEXANE	--	8	--	--	--	--	--	--
43271	2,4-DIMETHYLPENTANE	--	7	--	--	--	--	--	--
43278	2,5-DIMETHYLHEXANE	--	8	--	--	--	--	--	--
98110	2-(2-BUTOXYETHOXY)-ETHANOL	--	6	--	--	2	--	--	--
43308	2-BUTYLETHANOL	--	5	--	--	1	--	--	--
98108	2-BUTYLTETRAHYDROFURAN	--	7	--	--	1	--	--	--
98051	2-CHLOROTOLUENE	--	--	1	--	--	--	--	--
43311	2-ETHOXYETHANOL	--	2	--	--	--	1	--	--
43452	2-ETHOXYETHYL ACETATE	--	4	--	--	--	1	--	--
98002	2-ETHYL-1-BUTENE	--	5	--	--	1	--	--	--
98112	2-ETHYL-1-HEXANOL	--	7	--	--	1	--	--	--
43310	2-METHOXYETHANOL	--	1	--	--	--	1	--	--
43229	2-METHYL PENTANE	--	6	--	--	--	--	--	--
43225	2-METHYL-1-BUTENE	1	3	--	--	--	--	--	--
98040	2-METHYL-1-PENTENE	--	5	--	--	1	--	--	--
43228	2-METHYL-2-BUTENE	--	3	--	--	--	1	--	--
98004	2-METHYL-2-PENTENE	--	4	--	--	--	1	--	--
98076	2-METHYL-3-HEXANONE	--	7	--	--	--	--	--	--
43275	2-METHYLHEXANE	--	7	--	--	--	--	--	--

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
98032	3,5,5-TRIMETHYLHEXANE	--	9	--	--	--	--	--	--
98105	3-(CHLOROMETHYL)-HEPTANE	--	8	--	--	--	--	--	--
99021	3-CARENE	4	1	--	--	1	--	--	--
98041	3-HEPTENE	--	3	--	--	--	2	--	--
43230	3-METHYL PENTANE	--	6	--	--	--	--	--	--
43223	3-METHYL-1-BUTENE	1	3	--	--	--	--	--	--
43211	3-METHYL-1-PENTENE	1	4	--	--	--	--	--	--
43270	3-METHYL-T-2-PENTENE	--	4	--	--	--	1	--	--
43298	3-METHYLHEPTANE	--	8	--	--	--	--	--	--
43295	3-METHYLHEXANE	--	7	--	--	--	--	--	--
43293	4-METHYL-T-2-PENTENE	--	2	--	--	--	2	--	--
43297	4-METHYLHEPTANE	--	8	--	--	--	--	--	--
98042	4-NONENE	--	5	--	--	--	2	--	--
45221	A-METHYLSTYRENE	--	1	1	--	1	--	--	--
98025	A-PINENE	1	8	--	--	--	--	--	--
98097	A-TERPINEOL	1	6	--	--	--	1	--	--
43503	ACETALEHYDE	--	--	--	--	--	1	--	--
43404	ACETIC ACID	--	1	--	--	--	--	--	1
43551	ACETONE	--	3	--	--	--	--	--	--
43702	ACETONITRILE	--	1	--	--	--	--	--	1
43206	ACETYLENE	--	1	--	--	--	--	--	1
43505	ACROLEIN (ACRYLIC ALDHYDE)	1	--	--	--	1	--	--	--
43704	ACRYLONITRILE	1	1	--	--	--	--	--	--
98078	ALKENE KETONE	1	2	--	--	--	--	--	--
98085	ALKYL SUSTITUTED CYCLOHEXANE	--	9.5	--	--	--	--	--	--

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
99001	ALLYL CHLORIDE	1	1	--	--	--	--	--	--
98015	ANTHRACENE	--	6	--	1	--	--	--	--
98020	B-METHYLSTYRENE	--	--	1	--	--	1	--	--
98026	B-PINENE	1	8	--	--	--	--	--	--
45201	BENZENE	--	1	--	--	--	--	--	5
45402	BENZOIC ACID	--	--	1	--	--	--	--	--
98024	BENZYL CHLORIDE	--	--	1	--	--	--	--	--
99017	BROMODICHLOROMETHANE	--	--	--	--	--	--	--	1
99019	BROMOFORM	--	--	--	--	--	--	--	1
98080	BUTANDIOL	--	4	--	--	--	--	--	--
43213	BUTENE	1	2	--	--	--	--	--	--
98074	BUTYL CELLOSOLVE	--	4	--	--	--	1	--	--
43510	BUTYRALDEHYDE	--	2	--	--	--	1	--	--
98035	C-2-HEXENE	--	2	--	--	--	2	--	--
43266	C-2-OCTENE	--	6	--	--	2	--	--	--
98003	C-3-HEXENE	1	4	--	--	--	--	--	--
43115	C-7 CYCLOPARAFFINS	--	7	--	--	--	--	--	--
43116	C-8 CYCLOPARAFFINS	--	8	--	--	--	--	--	--
43117	C-9 CYCLOPARAFFINS	--	9	--	--	--	--	--	--
98050	C10 AROMATICS	--	3	1	--	--	--	--	--
98039	C10 OLEFINS	1	8	--	--	--	--	--	--
98086	C2 ALKYL DECALIN	--	12	--	--	--	--	--	--
98084	C2 ALKYL INDAN	--	4	1	--	--	--	--	--
98064	C2 CYCLOHEXANE	--	8	--	--	--	--	--	--

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
43511	C3 ALDEHYDE	--	1	--	--	--	1	--	--
98068	C3 ALKYL CYCLOHEXANE	--	9	--	--	--	--	--	--
98065	C3 CYCLOHEXANE	--	9	--	--	--	--	--	--
98069	C4 ALKYL CYCLOHEXANE	--	10	--	--	--	--	--	--
98066	C4 CYCLOHEXANE	--	10	--	--	--	--	--	--
98070	C4 SUBSTITUTED CYCLOHEXANE	--	10	--	--	--	--	--	--
98073	C4 SUBSTITUTED CYCLOHEXANONE	--	10	--	--	--	--	--	--
43512	C5 ALDEHYDE	--	3	--	--	--	1	--	--
98067	C5 CYCLOHEXANE	--	11	--	--	--	--	--	--
98075	C5 ESTER	--	7	--	--	--	--	--	--
98071	C5 SUBSTITUTED CYCLOHEXANE	--	11	--	--	--	--	--	--
98095	C6 ALDEHYDE	--	4	--	--	--	1	--	--
43289	C6 OLEFINS	1	4	--	--	--	--	--	--
98072	C6 SUBSTITUTED CYCLOHEXANE	--	12	--	--	--	--	--	--
98093	C7 ESTER	--	9	--	--	--	--	--	--
43294	C7-OLEFINS	1	5	--	--	--	--	--	--
43513	C8 ALDEHYDE	--	6	--	--	--	1	--	--
43290	C8 OLEFINS	1	6	--	--	--	--	--	--
98049	C9 AROMATICS	--	2	1	--	--	--	--	--
98038	C9 OLEFINS	1	7	--	--	--	--	--	--
98096	CARBITOL	--	2	--	--	--	2	--	--
98030	CARBON SULFIDE	--	1	--	--	--	--	--	--
43807	CARBON TETRABROMIDE	--	--	--	--	--	--	--	1
43804	CARBON TETRACHLORIDE	--	--	--	--	--	--	--	1
98031	CARBONYL SULFIDE	--	--	--	--	--	--	--	1

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
98087	CARVOMENTHOL	2	6	--	--	--	--	--	--
98088	CARVONE	2	6	--	--	--	--	--	--
43443	CELLOSOLVE ACETATE	--	3	--	--	--	1	--	1
99020	CHLORODIBROMOMETHANE	--	--	--	--	--	--	--	1
43825	CHLORODIFLUOROMETHANE (F-22)	--	--	--	--	--	--	--	1
43830	CHLOROFLUOROHYDROCARBONS	--	--	--	--	--	--	--	1
43803	CHLOROFORM	--	--	--	--	--	--	--	1
43827	CHLOROPENTAFLUOROETHANE(F-115)	--	--	--	--	--	--	--	2
99003	CHLOROPRENE	2	--	--	--	--	--	--	--
43826	CHLOROTRIFLUOROMETHANE (F-13)	--	--	--	--	--	--	--	1
43217	CIS-2-BUTENE	--	--	--	--	--	2	--	--
43227	CIS-2-PENTENE	--	1	--	--	--	2	--	--
98019	CRYOFLOURANE (F 114)	--	--	--	--	--	--	--	2
43248	CYCLOHEXANE	--	6	--	--	--	--	--	--
43264	CYCLOHEXANONE	--	6	--	--	--	--	--	--
43273	CYCLOHEXENE	1	4	--	--	--	--	--	--
43242	CYCLOPENTANE	--	5	--	--	--	--	--	--
43292	CYCLOPENTENE	1	3	--	--	--	--	--	--
43207	CYCLOPROPANE	--	3	--	--	--	--	--	--
98027	D-LIMONENE	1	4	--	--	--	2	--	--
43320	DIACETONE ALCOHOL	--	4	--	--	--	1	--	--
99015	DIBENZOFURAN	--	2	2	--	--	--	--	--
98107	DIBUTYL ETHER	--	6	--	--	--	1	--	--
43823	DICHLORODIFLOUROMETHANE (F-12)	--	--	--	--	--	--	--	1
43802	DICHLOROMETHANE	--	--	--	--	--	--	--	1

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
43828	DICHLOROTETRAFLUOROETHANE/114	--	--	--	--	--	--	--	2
98062	DIETHYLCYCLOHEXANE	--	10	--	--	--	--	--	--
98018	DIMETHYL ETHER	--	2	--	--	--	--	--	--
43450	DIMETHYL FORMAMIDE	--	--	--	--	--	--	--	3
98059	DIMETHYLCYCLOHEXANE	--	8	--	--	--	--	--	--
45103	DIMETHYLETHYLBENZENE	--	2	--	1	--	--	--	--
98091	DIMETHYLHEPTANE	--	9	--	--	--	--	--	--
98012	DIMETHYLNAPHTHALENE	--	4	--	1	--	--	--	--
98017	DM-2,3,DH-1H-INDENE	--	3	--	1	--	--	--	--
43287	DOCOSANE	--	22	--	--	--	--	--	--
43285	EICOSANE	--	20	--	--	--	--	--	--
99006	EPICHLOROHYDRIN	--	3	--	--	--	--	--	--
43202	ETHANE	--	0.4	--	--	--	--	--	1.6
43433	ETHYL ACETATE	--	3	--	--	--	--	--	1
43438	ETHYL ACRYLATE	--	1	--	--	--	2	--	--
43302	ETHYL ALCOHOL	--	2	--	--	--	--	--	--
43812	ETHYL CHLORIDE	--	--	--	--	--	--	--	2
43351	ETHYL ETHER	--	2	--	--	--	1	--	--
98106	ETHYL ISOPROPYL ETHER	--	3	--	--	--	1	--	--
43219	ETHYLACETYLENE	--	4	--	--	--	--	--	--
43721	ETHYLAMINE	--	1	--	--	--	--	--	1
45203	ETHYLBENZENE	--	1	1	--	--	--	--	--
43288	ETHYLCYCLOHEXANE	--	8	--	--	--	--	--	--
98061	ETHYLCYCLOHEXANE	--	8	--	--	--	--	--	--
98057	ETHYLCYCLOPENTANE	--	7	--	--	--	--	--	--

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
43203	ETHYLENE	--	--	--	--	--	--	1	--
99014	ETHYLENE DIBROMIDE	--	2	--	--	--	--	--	--
43815	ETHYLENE DICHLORIDE	--	--	--	--	--	--	1	--
43370	ETHYLENE GLYCOL	--	2	--	--	--	--	--	--
43601	ETHYLENE OXIDE	--	1	--	--	--	--	--	1
98082	ETHYLHEPTENE	1	7	--	--	--	--	--	--
98011	ETHYLNAPHTHALENE	--	5	1	--	--	--	--	--
43502	FORMALDEHYDE	--	--	--	--	1	--	--	--
43368	GLYCOL	--	2	--	--	--	--	--	--
43367	GLYCOL ETHER	--	2	--	--	--	--	--	--
43286	HENEICOSANE	--	21	--	--	--	--	--	--
43282	HEPTADECANE	--	17	--	--	--	--	--	--
43232	HEPTANE	--	7	--	--	--	--	--	--
98077	HEPTANONE	--	7	--	--	--	--	--	--
99007	HEXACHLOROCYCLOPENTADIENE	1	3	--	--	--	--	--	--
43281	HEXADECANE	--	16	--	--	--	--	--	--
43231	HEXANE	--	6	--	--	--	--	--	--
43371	HEXYLENE GLYCOL	--	6	--	--	--	--	--	--
98044	INDAN	--	2	1	--	--	--	--	--
98048	INDENE	1	--	1	--	--	--	--	--
98115	ISOAMYL ISOBUTYRATE	--	9	--	--	--	--	--	--
43214	ISOBUTANE	--	4	--	--	--	--	--	--
43446	ISOBUTYL ACETATE	--	6	--	--	--	--	--	--
43306	ISOBUTYL ALCOHOL	--	4	--	--	--	--	--	--
43451	ISOBUTYL ISOBUTYRATE	--	6	--	--	--	1	--	--

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
98047	ISOBUTYLBENZENE	--	3	1	--	--	--	--	--
43215	ISOBUTYLENE	--	1	--	--	1	1	--	--
98036	ISOBUTYRALDEHYDE	--	2	--	--	--	2	--	--
43120	ISOMERS OF BUTENE	--	--	--	--	--	2	--	--
45105	ISOMERS OF BUTYLBENZENE	--	3	1	--	--	--	--	--
43109	ISOMERS OF DECANE	--	10	--	--	--	--	--	--
45106	ISOMERS OF DIETHYLBENZENE	--	2	--	1	--	--	--	--
43112	ISOMERS OF DODECANE	--	12	--	--	--	--	--	--
45104	ISOMERS OF ETHYLTOLUENE	--	1	--	1	--	--	--	--
43106	ISOMERS OF HEPTANE	--	7	--	--	--	--	--	--
43105	ISOMERS OF HEXANE	--	6	--	--	--	--	--	--
43108	ISOMERS OF NONANE	--	9	--	--	--	--	--	--
43107	ISOMERS OF OCTANE	--	8	--	--	--	--	--	--
43114	ISOMERS OF PENTADECANE	--	15	--	--	--	--	--	--
43122	ISOMERS OF PENTANE	--	5	--	--	--	--	--	--
43121	ISOMERS OF PENTENE	--	1	--	--	--	2	--	--
43113	ISOMERS OF TETRADECANE	--	14	--	--	--	--	--	--
43111	ISOMERS OF TRIDECANE	--	13	--	--	--	--	--	--
43110	ISOMERS OF UNDECANE	--	11	--	--	--	--	--	--
45102	ISOMERS OF XYLENE	--	--	--	1	--	--	--	--
43243	ISOPRENE	2	1	--	--	--	--	--	--
43444	ISOPROPYL ACETATE	--	5	--	--	--	--	--	--
43304	ISOPROPYL ALCOHOL	--	3	--	--	--	--	--	--
98043	ISOPROPYLBENZENE (CUMENE)	--	2	1	--	--	--	--	--
98089	ISOPULEGONE	1	8	--	--	--	--	--	--

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
98056	ISOVALERALDEHYDE	--	3	--	--	--	1	--	--
43119	LACTOL SPIRITS	--	8	--	--	--	--	--	--
98022	M-CRESOL (3-M-BENZENOL)	--	--	1	--	--	--	--	--
98045	M-DIETHYLBENZENE	--	2	--	1	--	--	--	--
45212	M-ETHYLTOLUENE	--	1	--	1	--	--	--	--
45205	M-XYLENE	--	--	--	1	--	--	--	--
99008	MALEIC ANHYDRIDE	1	2	--	--	--	--	--	--
43201	METHANE	--	0.01	--	--	--	--	--	0.99
43432	METHYL ACETATE	--	--	--	--	--	--	--	3
43301	METHYL ALCOHOL	--	1	--	--	--	--	--	--
43445	METHYL AMYL ACETATE	--	8	--	--	--	--	--	--
43561	METHYL AMYL KETONE	--	7	--	--	--	--	--	--
43819	METHYL BROMIDE	--	--	--	--	--	--	--	1
43801	METHYL CHLORIDE	--	--	--	--	--	--	--	1
43552	METHYL ETHYL KETONE	--	4	--	--	--	--	--	--
98090	METHYL HEPTENE	1	6	--	--	--	--	--	--
43560	METHYL ISOBUTYL KETONE	--	6	--	--	--	--	--	--
98114	METHYL ISOBUTYRATE	--	5	--	--	--	--	--	--
43559	METHYL N-BUTYL KETONE	--	6	--	--	--	--	--	--
43209	METHYLACETYLENE	--	1.5	--	--	--	--	--	1.5
98016	METHYLANTHRACENE	--	9	--	1	--	--	--	--
43261	METHYLCYCLOHEXANE	--	7	--	--	--	--	--	--
43262	METHYLCYCLOPENTANE	--	6	--	--	--	--	--	--
43272	METHYLCYCLOPENTENE	1	4	--	--	--	--	--	--
43805	METHYLENE BROMIDE	--	--	--	--	--	--	--	1

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
98010	METHYLNAPHTHALENE	--	3	--	1	--	--	--	--
45234	METHYLPROPYLBENZENE	--	2	--	1	--	--	--	--
43118	MINERAL SPIRITS	--	6	--	--	--	1	--	--
45801	MONOCHLOROBENZENE	--	5	--	--	--	--	--	1
43212	N-BUTANE	--	4	--	--	--	--	--	--
43435	N-BUTYL ACETATE	--	5	--	--	--	--	--	1
43305	N-BUTYL ALCOHOL	--	2	--	--	--	1	--	--
43238	N-DECANE	--	10	--	--	--	--	--	--
43255	N-DODECANE	--	12	--	--	--	--	--	--
43260	N-PENTADECANE	--	15	--	--	--	--	--	--
43220	N-PENTANE	--	5	--	--	--	--	--	--
98063	N-PENTYLCYCLOHEXANE	--	11	--	--	--	--	--	--
43303	N-PROPYL ALCOHOL	--	3	--	--	--	--	--	--
45209	N-PROPYLBENZENE	--	2	1	--	--	--	--	--
43259	N-TETRADECANE	--	14	--	--	--	--	--	--
43258	N-TRIDECANE	--	13	--	--	--	--	--	--
45101	NAPHTHA	--	8	--	--	--	--	--	--
98046	NAPHTHALENE	--	2	--	1	--	--	--	--
99009	NITROBENZENE	--	1	--	--	--	--	--	5
99010	NITROSOMORPHOLINE	--	3	--	--	1	--	--	--
43284	NONADECANE	--	19	--	--	--	--	--	--
43235	NONANE	--	9	--	--	--	--	--	--
98021	O-CRESOL (2-M-BENZENOL)	--	--	1	--	--	--	--	--
45211	O-ETHYLTOLUENE	--	1	--	1	--	--	--	--
45204	O-XYLENE	--	--	--	1	--	--	--	--

TABLE B-2. (continued)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
43283	OCTADECANE	--	18	--	--	--	--	--	--
43233	OCTANE	--	8	--	--	--	--	--	--
43265	OCTENE	1	6	--	--	--	--	--	--
98023	P-CRESOL (4-M-BENZENOL)	--	--	1	--	--	--	--	--
45807	P-DICHLOROBENZENE	--	5	--	--	--	--	--	1
45206	P-XYLENE	--	--	--	1	--	--	--	--
98094	PENTYL ALCOHOL	--	4	--	--	1	--	--	--
43817	PERCHLOROETHYLENE	--	--	--	--	--	--	--	2
45300	PHENOLS	--	--	--	--	--	1	--	4
43850	PHOSGENE (CCL2O)	--	--	--	--	1	--	--	--
98028	PHTHALIC ANAHYDRIDE	--	--	--	1	--	--	--	2
43208	PROPADIENE	--	--	--	--	1	1	--	--
43204	PROPANE	--	1.5	--	--	--	--	--	1.5
43504	PROPRIONALDEHYDE	--	1	--	--	--	1	--	--
43434	PROPYL ACETATE	--	4	--	--	--	--	--	1
45108	PROPYLBENZENE	--	2	1	--	--	--	--	--
98109	PROPYLCYCLOHEXANONE	--	9	--	--	--	--	--	--
43205	PROPYLENE	1	1	--	--	--	--	--	--
43369	PROPYLENE GLYCOL	--	3	--	--	--	--	--	--
43602	PROPYLENE OXIDE	--	2	--	--	--	--	--	1
98013	PROPYLNAPHTHALENE	--	6	1	--	--	--	--	--
45216	SEC-BUTYLBENZENE	--	3	1	--	--	--	--	--
45220	STYRENE	--	--	1	--	1	--	--	--
98116	SUBSTITUTED C7 ESTER (C12)	--	9	--	--	1	--	--	2
98117	SUBSTITUTED C9 ESTER (C12)	--	10	--	--	1	--	--	1

TABLE B-2. (concluded)

SAROAD Code	Chemical Name	OLE	PAR	TOL	XYL	FORM	ALD2	ETH	NR
98034	T-2-HEXENE	--	2	--	--	--	2	--	--
98052	T-BUTYLBENZENE	--	3	1	--	--	--	--	--
43123	TERPENES	1	8	--	--	--	--	--	--
98079	TERPINENE	2	6	--	--	--	--	--	--
43309	TERT-BUTYL ALCOHOL	--	--	--	--	--	--	--	4
45215	TERT-BUTYLBENZENE	--	1	1	--	--	--	--	3
43390	TETRAHYDROFURAN	--	3	--	--	1	--	--	--
45232	TETRAMETHYLBENZENE	--	2	--	1	--	--	--	--
45202	TOLUENE	--	--	1	--	--	--	--	--
99018	TRANS-1,2-DICHLOROETHENE	--	--	--	--	--	--	1	--
43216	TRANS-2-BUTENE	--	--	--	--	--	2	--	--
43226	TRANS-2-PENTENE	--	1	--	--	--	2	--	--
45233	TRI/TETRAALKYL BENZENE	--	3	--	1	--	--	--	--
43824	TRICHLOROETHYLENE	--	--	--	--	--	--	1	--
43811	TRICHLOROFLOUROMETHANE	--	--	--	--	--	--	--	1
43821	TRICHLOROTRIFLOUROETHANE	--	--	--	--	--	--	--	2
43740	TRIMETHYL AMINE	--	3	--	--	--	--	--	--
45107	TRIMETHYLBENZENE	--	1	--	1	--	--	--	--
98060	TRIMETHYLCYCLOHEXANE	--	9	--	--	--	--	--	--
98058	TRIMETHYLCYCLOPENTANE	--	8	--	--	--	--	--	--
98083	TRIMETHYLDECENE	1	11	--	--	--	--	--	--
43822	TRIMETHYLFLUOROSILANE	--	--	--	--	--	--	--	3
98014	TRIMETHYLNAPHTHALENE	--	5	--	1	--	--	--	--
43241	UNDECANE	--	11	--	--	--	--	--	--
43860	VINYL CHLORIDE	--	--	--	--	--	--	1	--
45401	XYLENE BASE ACIDS	--	--	--	1	--	--	--	--